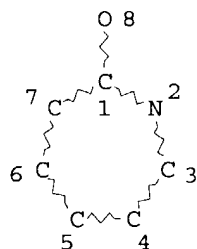


=> d que 1103

L96 STR



NODE ATTRIBUTES:

CONNECT IS E1 RC AT 8
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

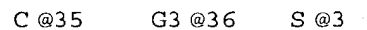
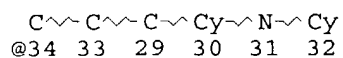
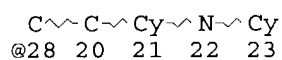
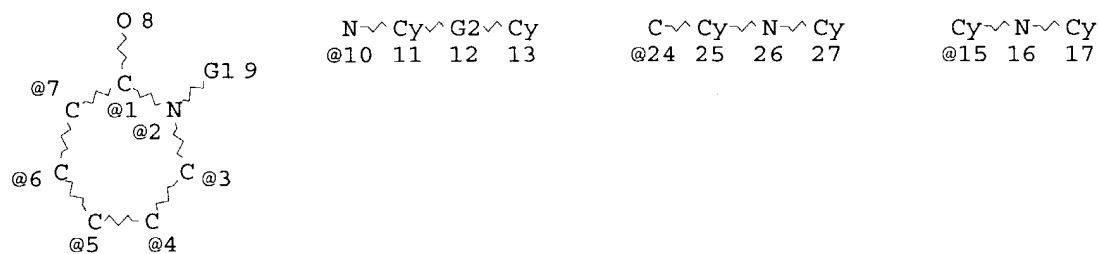
GRAPH ATTRIBUTES:

RSPEC I
 NUMBER OF NODES IS 8

STEREO ATTRIBUTES: NONE

L97 17246 SEA FILE=REGISTRY SSS FUL L96

L101 STR



C @38

Page 1-A

7

Page 1-B

VAR G1=15/10/24/28/34

REP G2=(0-4) 35

VAR G3=37/38

VPA 36-1/2/3/4/5/6/7 U

NODE ATTRIBUTES:

NSPEC IS RC AT 10
 NSPEC IS RC AT 16
 NSPEC IS RC AT 20
 NSPEC IS RC AT 22

NSPEC IS RC AT 24
NSPEC IS RC AT 26
NSPEC IS RC AT 28
NSPEC IS RC AT 29
NSPEC IS RC AT 31
NSPEC IS RC AT 33
NSPEC IS RC AT 34
NSPEC IS RC AT 35
NSPEC IS RC AT 37
NSPEC IS RC AT 38
CONNECT IS E1 RC AT 8
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC 2
NUMBER OF NODES IS 35

STEREO ATTRIBUTES: NONE

L103 0 SEA FILE=REGISTRY SUB=L97 SSS FUL L101

=> fil lreg

FILE 'LREGISTRY' ENTERED AT 09:25:00 ON 03 DEC 2004
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LREGISTRY IS A STATIC LEARNING FILE

=> fil reg

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STRUCTURE FILE UPDATES: 1 DEC 2004 HIGHEST RN 791553-15-6
DICTIONARY FILE UPDATES: 1 DEC 2004 HIGHEST RN 791553-15-6

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when
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Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

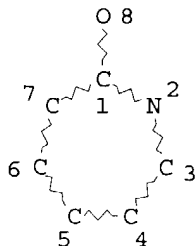
=> file stnguide

FILE 'STNGUIDE' ENTERED AT 09:25:05 ON 03 DEC 2004
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FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Nov 26, 2004 (20041126/UP).

=> d que 174

L58 STR



NODE ATTRIBUTES:
CONNECT IS E1 RC AT 8
DEFAULT MLEVEL IS ATOM

case I

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

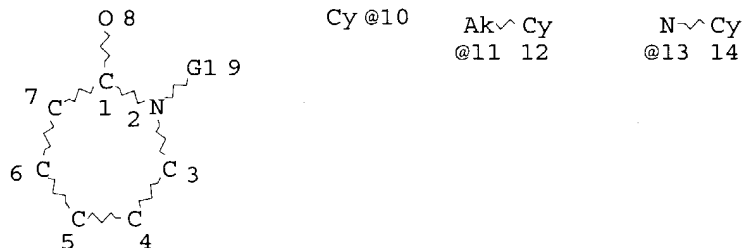
RSPEC I

NUMBER OF NODES IS 8

STEREO ATTRIBUTES: NONE

L59 (17246)SEA FILE=REGISTRY SSS FUL L58

L60 STR



VAR G1=10/11/13

NODE ATTRIBUTES:

CONNECT IS E1 RC AT 8

DEFAULT MLEVEL IS ATOM

GGCAT IS PCY AT 10

GGCAT IS PCY AT 12

GGCAT IS PCY AT 14

DEFAULT ECLEVEL IS LIMITED

ECOUNT IS X9 C AT 11

GRAPH ATTRIBUTES:

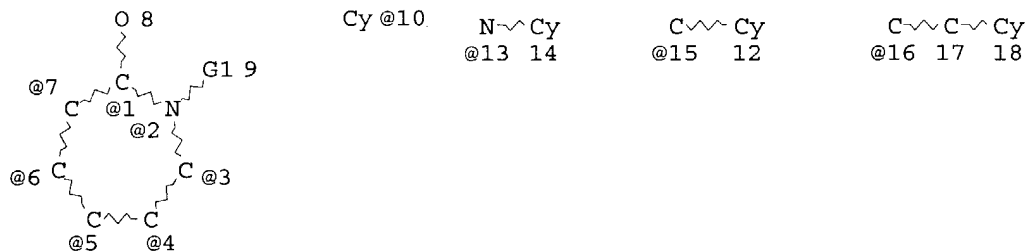
RSPEC 2

NUMBER OF NODES IS 14

STEREO ATTRIBUTES: NONE

L61 141 SEA FILE=REGISTRY SUB=L59 SSS FUL L60

L72 STR



C ~ C ~ C ~ Cy
@19 20 21 22

A @23

VAR G1=10/13/15/16/19

VPA 23-1/2/3/4/5/6/7 U

NODE ATTRIBUTES:

NSPEC IS RC AT 13

NSPEC IS RC AT 15

NSPEC IS RC AT 16

NSPEC IS RC AT 17

NSPEC IS RC AT 19
NSPEC IS RC AT 20
NSPEC IS RC AT 21
NSPEC IS RC AT 23
CONNECT IS E1 RC AT 8
DEFAULT MLEVEL IS ATOM
GGCAT IS PCY AT 10
GGCAT IS PCY AT 12
GGCAT IS PCY AT 14
GGCAT IS PCY AT 18
GGCAT IS PCY AT 22
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC 2
NUMBER OF NODES IS 22

STEREO ATTRIBUTES: NONE

L74 29 SEA FILE=REGISTRY SUB=L61 SSS FUL L72

=> fil reg

FILE 'REGISTRY' ENTERED AT 09:25:23 ON 03 DEC 2004
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STRUCTURE FILE UPDATES: 1 DEC 2004 HIGHEST RN 791553-15-6
DICTIONARY FILE UPDATES: 1 DEC 2004 HIGHEST RN 791553-15-6

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> analyze l74

ENTER ANSWER NUMBER OR RANGE (1-):1-
ENTER DISPLAY CODE (CHEM) OR ?:lc
L75 ANALYZE L74 1- LC : 9 TERMS

=> d

L75 ANALYZE L74 1- LC : 9 TERMS

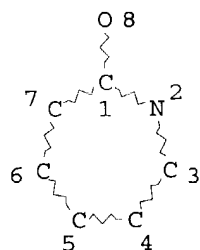
TERM #	# OCC	# DOC	% DOC LC
1	27	27	93.10 CA
2	27	27	93.10 CAPLUS
3	14	14	48.28 USPATFULL
4	10	10	34.48 TOXCENTER

***** END OF L75***

FILE 'STNGUIDE' ENTERED AT 09:25:47 ON 03 DEC 2004
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FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Nov 26, 2004 (20041126/UP).

=> => d que 185
L62 STR



Case II

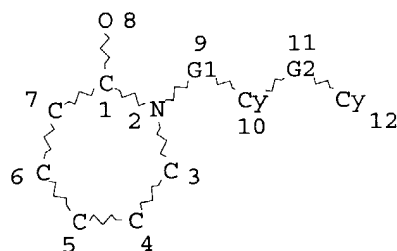
```

NODE ATTRIBUTES:
CONNECT IS E1 RC AT 8
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

```

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 8

```
STEREO ATTRIBUTES: NONE
L63 (      17246)SEA FILE=REGISTRY SSS FUL L62
L64          STR
```



C @13 C @14

```

REP G1=(0-6) 13
REP G2=(0-6) 14
NODE ATTRIBUTES:
NSPEC      IS RC      AT      13
NSPEC      IS RC      AT      14
CONNECT IS E1  RC AT      8

```

DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

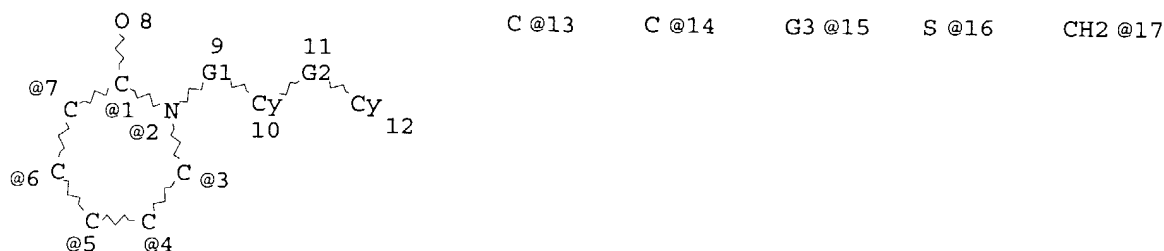
RSPEC 2

NUMBER OF NODES IS 14

STEREO ATTRIBUTES: NONE

L65 647 SEA FILE=REGISTRY SUB=L63 SSS FUL L64

L79 STR



REP G1=(0-4) 13

REP G2=(0-4) 14

VAR G3=16/17

VPA 15-1/2/3/4/5/6/7 U

NODE ATTRIBUTES:

NSPEC IS RC AT 13

NSPEC IS RC AT 14

NSPEC IS RC AT 16

CONNECT IS E1 RC AT 8

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC 2

NUMBER OF NODES IS 17

STEREO ATTRIBUTES: NONE

L85 86 SEA FILE=REGISTRY SUB=L65 SSS FUL L79

=>

=> fil reg

FILE 'REGISTRY' ENTERED AT 09:53:16 ON 03 DEC 2004

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STRUCTURE FILE UPDATES: 1 DEC 2004 HIGHEST RN 791553-15-6

DICTIONARY FILE UPDATES: 1 DEC 2004 HIGHEST RN 791553-15-6

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

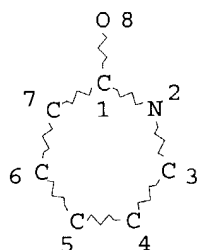
```
=> analyze l85
ENTER ANSWER NUMBER OR RANGE (1-):1-
ENTER DISPLAY CODE (CHEM) OR ?:lc
L86          ANALYZE L85 1- LC :          3 TERMS
```

```
=> d
L86          ANALYZE L85 1- LC :          3 TERMS
```

TERM #	# OCC	# DOC	% DOC	LC
1	86	86	100.00	CA
2	86	86	100.00	CAPLUS
3	30	30	34.88	USPATFULL

***** END OF L86***

```
=> d que l69
L66          STR
```

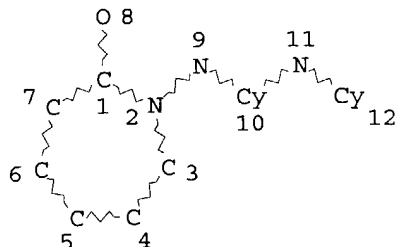


case III

NODE ATTRIBUTES:
CONNECT IS E1 RC AT 8
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 8

STEREO ATTRIBUTES: NONE
L67 (17246)SEA FILE=REGISTRY SSS FUL L66
L68 STR



NODE ATTRIBUTES:

NSPEC IS RC AT 9
NSPEC IS RC AT 11
CONNECT IS E1 RC AT 8
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC 2
NUMBER OF NODES IS 12

STEREO ATTRIBUTES: NONE

L69 0 SEA FILE=REGISTRY SUB=L67 SSS FUL L68

=> file stnguide

FILE 'STNGUIDE' ENTERED AT 09:53:52 ON 03 DEC 2004
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FILE CONTAINS CURRENT INFORMATION.

LAST RELOADED: Nov 26, 2004 (20041126/UP).

=> => fil hcap

FILE 'HCAPLUS' ENTERED AT 10:00:06 ON 03 DEC 2004
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FILE COVERS 1907 - 3 Dec 2004 VOL 141 ISS 23
FILE LAST UPDATED: 1 Dec 2004 (20041201/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> fil uspatfull

FILE 'USPATFULL' ENTERED AT 10:00:10 ON 03 DEC 2004
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FILE COVERS 1971 TO PATENT PUBLICATION DATE: 2 Dec 2004 (20041202/PD)
FILE LAST UPDATED: 2 Dec 2004 (20041202/ED)
HIGHEST GRANTED PATENT NUMBER: US6826778
HIGHEST APPLICATION PUBLICATION NUMBER: US2004244085
CA INDEXING IS CURRENT THROUGH 2 Dec 2004 (20041202/UPCA)

ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 2 Dec 2004 (20041202/PD)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Aug 2004
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Aug 2004

```
>>> USPAT2 is now available. USPATFULL contains full text of the <<<
>>> original, i.e., the earliest published granted patents or <<<
>>> applications. USPAT2 contains full text of the latest US <<<
>>> publications, starting in 2001, for the inventions covered in <<<
>>> USPATFULL. A USPATFULL record contains not only the original <<<
>>> published document but also a list of any subsequent <<<
>>> publications. The publication number, patent kind code, and <<<
>>> publication date for all the US publications for an invention <<<
>>> are displayed in the PI (Patent Information) field of USPATFULL <<<
>>> records and may be searched in standard search fields, e.g., /PN, <<<
>>> /PK, etc. <<<

>>> USPATFULL and USPAT2 can be accessed and searched together <<<
>>> through the new cluster USPATALL. Type FILE USPATALL to <<<
>>> enter this cluster. <<<
>>> Use USPATALL when searching terms such as patent assignees, <<<
>>> classifications, or claims, that may potentially change from <<<
>>> the earliest to the latest publication. <<<
```

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> fil casreact

FILE 'CASREACT' ENTERED AT 10:00:13 ON 03 DEC 2004
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FILE CONTENT:1840 - 28 Nov 2004 VOL 141 ISS 22

```
*****
*
*      CASREACT now has more than 8 million reactions
*
*****
```

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> fil toxcenter

FILE 'TOXCENTER' ENTERED AT 10:00:17 ON 03 DEC 2004
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FILE COVERS 1907 TO 30 Nov 2004 (20041130/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

TOXCENTER has been enhanced with new files segments and search fields.
See HELP CONTENT for more information.

TOXCENTER thesauri in the /CN, /CT, and /MN fields incorporate the MeSH 2004 vocabulary. See <http://www.nlm.nih.gov/mesh/> and http://www.nlm.nih.gov/pubs/techbull/nd03/nd03_mesh.html for a description of changes.

=> file stnguide

FULL ESTIMATED COST 0.61 374.71

FILE 'STNGUIDE' ENTERED AT 10:00:22 ON 03 DEC 2004
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FILE CONTAINS CURRENT INFORMATION.

LAST RELOADED: Nov 26, 2004 (20041126/UP).

=> d que nos 189

L58 STR
L59 (17246)SEA FILE=REGISTRY SSS FUL L58
L60 STR
L61 141 SEA FILE=REGISTRY SUB=L59 SSS FUL L60
L62 STR
L63 (17246)SEA FILE=REGISTRY SSS FUL L62
L64 STR
L65 647 SEA FILE=REGISTRY SUB=L63 SSS FUL L64
L72 STR
L74 29 SEA FILE=REGISTRY SUB=L61 SSS FUL L72
L79 STR
L85 86 SEA FILE=REGISTRY SUB=L65 SSS FUL L79
L87 19 SEA FILE=HCAPLUS ABB=ON PLU=ON L74
L88 4 SEA FILE=HCAPLUS ABB=ON PLU=ON L85
L89 22 SEA FILE=HCAPLUS ABB=ON PLU=ON L87 OR L88

=> d que nos 192

L58 STR
L59 (17246)SEA FILE=REGISTRY SSS FUL L58
L60 STR
L61 141 SEA FILE=REGISTRY SUB=L59 SSS FUL L60
L62 STR
L63 (17246)SEA FILE=REGISTRY SSS FUL L62
L64 STR
L65 647 SEA FILE=REGISTRY SUB=L63 SSS FUL L64
L72 STR
L74 29 SEA FILE=REGISTRY SUB=L61 SSS FUL L72
L79 STR
L85 86 SEA FILE=REGISTRY SUB=L65 SSS FUL L79
L90 6 SEA FILE=USPATFULL ABB=ON PLU=ON L74
L91 1 SEA FILE=USPATFULL ABB=ON PLU=ON L85
L92 7 SEA FILE=USPATFULL ABB=ON PLU=ON (L90 OR L91)

=> d que nos 193

L58 STR
L59 (17246) SEA FILE=REGISTRY SSS FUL L58
L60 STR
L61 141 SEA FILE=REGISTRY SUB=L59 SSS FUL L60
L62 STR
L63 (17246) SEA FILE=REGISTRY SSS FUL L62
L64 STR
L65 647 SEA FILE=REGISTRY SUB=L63 SSS FUL L64
L72 STR
L74 29 SEA FILE=REGISTRY SUB=L61 SSS FUL L72
L79 STR
L85 86 SEA FILE=REGISTRY SUB=L65 SSS FUL L79
L93 2 SEA FILE=CASREACT ABB=ON PLU=ON L74 OR L85

=> d que nos 194

L58 STR
L59 (17246) SEA FILE=REGISTRY SSS FUL L58
L60 STR
L61 141 SEA FILE=REGISTRY SUB=L59 SSS FUL L60
L62 STR
L63 (17246) SEA FILE=REGISTRY SSS FUL L62
L64 STR
L65 647 SEA FILE=REGISTRY SUB=L63 SSS FUL L64
L72 STR
L74 29 SEA FILE=REGISTRY SUB=L61 SSS FUL L72
L79 STR
L85 86 SEA FILE=REGISTRY SUB=L65 SSS FUL L79
L94 10 SEA FILE=TOXCENTER ABB=ON PLU=ON L74 OR L85

=> dup rem 189 192 193 194

FILE 'HCAPLUS' ENTERED AT 10:01:06 ON 03 DEC 2004
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FILE 'CASREACT' ENTERED AT 10:01:06 ON 03 DEC 2004
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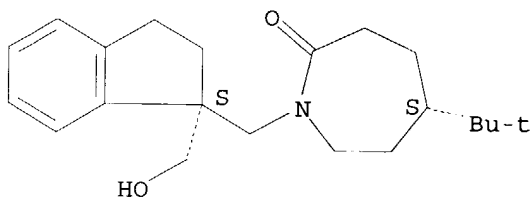
FILE 'TOXCENTER' ENTERED AT 10:01:06 ON 03 DEC 2004
COPYRIGHT (C) 2004 ACS
PROCESSING COMPLETED FOR L89
PROCESSING COMPLETED FOR L92
PROCESSING COMPLETED FOR L93
PROCESSING COMPLETED FOR L94
L95 30 DUP REM L89 L92 L93 L94 (11 DUPLICATES REMOVED)
ANSWERS '1-21' FROM FILE HCAPLUS
ANSWERS '22-26' FROM FILE USPATFULL
ANSWERS '27-30' FROM FILE TOXCENTER

=> d ibib abs ed hitstr 1-21

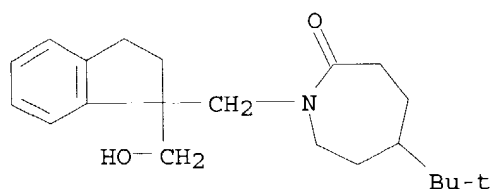
L95 ANSWER 1 OF 30 HCAPLUS COPYRIGHT 2004 ACS on STN DUPLICATE 1
ACCESSION NUMBER: 2003:837735 HCAPLUS

DOCUMENT NUMBER: 140:59238
TITLE: Unusual Tethering Effects in the Schmidt Reaction of Hydroxyalkyl Azides with Ketones: Cation- π and Steric Stabilization of a Pseudoaxial Phenyl Group
AUTHOR(S): Katz, Christopher E.; Aube, Jeffrey
CORPORATE SOURCE: Department of Chemistry, University of Kansas, Lawrence, KS, 66045-7582, USA
SOURCE: Journal of the American Chemical Society (2003), 125(46), 13948-13949
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:59238
AB The Lewis acid-promoted reactions of chiral 2-aryl-3-azido-1-propanols with 4-substituted cyclohexanones lead to iminium ethers and ultimately caprolactams (following a hydrolysis step). In this study, it is shown that these reactions afford variable ratios of products, depending on the electronic nature of the Ph group. These results are interpreted in the context of a cation- π stabilizing effect in the product-determining reaction intermediate. Remarkably, the best selectivity was obtained when an azidopropanol reagent containing a quaternary center was used; a control experiment showed that the high selectivity observed in this result depended upon the free rotation of the pseudoaxial aromatic group in the intermediate that affords the major product.
ED Entered STN: 27 Oct 2003
IT 637357-23-4P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (unusual tethering effects in Schmidt reaction of hydroxyalkyl azides with ketones)
RN 637357-23-4 HCAPLUS
CN 2H-Azepin-2-one, 1-[[[(1R)-2,3-dihydro-1-(hydroxymethyl)-1H-inden-1-yl]methyl]-5-(1,1-dimethylethyl)hexahydro-, (5R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

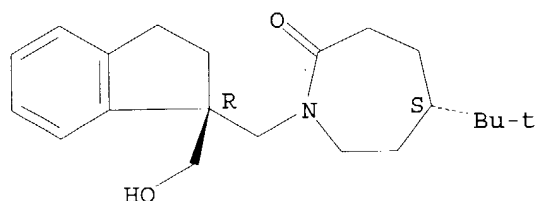


IT 637356-71-9P 637356-73-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (unusual tethering effects in Schmidt reaction of hydroxyalkyl azides with ketones)
RN 637356-71-9 HCAPLUS
CN 2H-Azepin-2-one, 1-[[[2,3-dihydro-1-(hydroxymethyl)-1H-inden-1-yl]methyl]-5-(1,1-dimethylethyl)hexahydro- (9CI) (CA INDEX NAME)



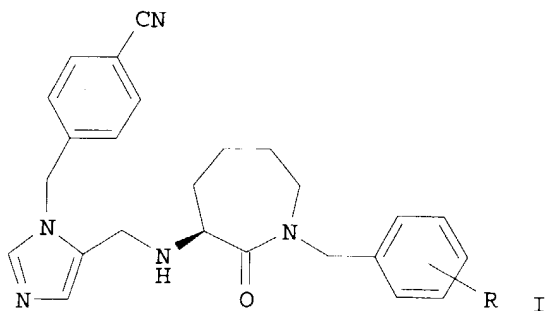
RN 637356-73-1 HCAPLUS
 CN 2H-Azepin-2-one, 1-[[[(1R)-2,3-dihydro-1-(hydroxymethyl)-1H-inden-1-yl]methyl]-5-(1,1-dimethylethyl)hexahydro-, (5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L95 ANSWER 2 OF 30 HCAPLUS COPYRIGHT 2004 ACS on STN DUPLICATE 2
 ACCESSION NUMBER: 2003:462563 HCAPLUS
 DOCUMENT NUMBER: 140:42082
 TITLE: Parallel liquid synthesis of N,N'-disubstituted 3-aminoazepin-2-ones as potent and specific farnesyl transferase inhibitors
 AUTHOR(S): Le Diguarher, Thierry; Ortuno, Jean-Claude; Dorey, Gilbert; Shanks, David; Guilbaud, Nicolas; Pierre, Alain; Fauchere, Jean-Luc; Hickman, John A.; Tucker, Gordon C.; Casara, Patrick J.
 CORPORATE SOURCE: Department of Medicinal Chemistry, Institut de Recherches Servier, Croissy sur Seine, 78290, Fr.
 SOURCE: Bioorganic & Medicinal Chemistry (2003), 11(14), 3193-3204
 CODEN: BMECEP; ISSN: 0968-0896
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 140:42082
 GI



AB A rapid structure-activity study was performed by parallel liquid synthesis on N,N'-disubstitution of 3-aminoazepin-2-one to afford potent and specific farnesyl transferase inhibitors with low nM enzymic and cellular activities. The activities of the selected compds. were validated in vivo, and compds. I (R = 2-Cl, 3-Br) presented significant antitumor activity.

ED Entered STN: 17 Jun 2003

IT **635753-79-6P**

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(N,N'-disubstituted 3-aminoazepin-2-ones as farnesyl transferase inhibitors)

RN 635753-79-6 HCAPLUS

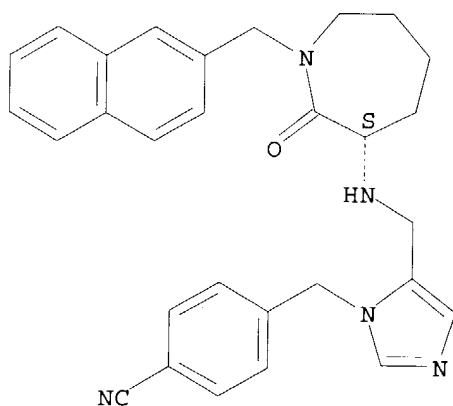
CN Benzonitrile, 4-[[[5-[[[(3S)-hexahydro-1-(2-naphthalenylmethyl)-2-oxo-1H-azepin-3-yl]amino]methyl]-1H-imidazol-1-yl]methyl]-, (2E)-2-butenedioate (9CI) (CA INDEX NAME)

CM 1

CRN 443920-60-3

CMF C29 H29 N5 O

Absolute stereochemistry.

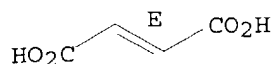


CM 2

CRN 110-17-8

CMF C4 H4 O4

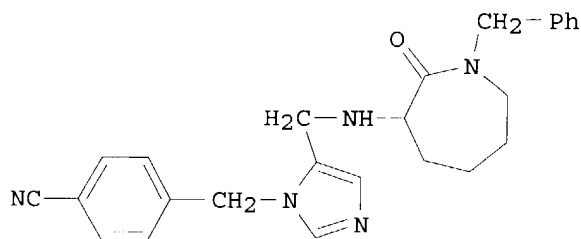
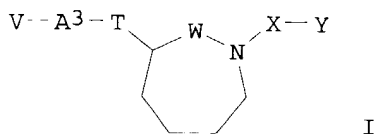
Double bond geometry as shown.



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L95 ANSWER 3 OF 30 HCAPLUS COPYRIGHT 2004 ACS on STN DUPLICATE 3
 ACCESSION NUMBER: 2002:555454 HCAPLUS
 DOCUMENT NUMBER: 137:125097
 TITLE: Novel azepanes as farnesyl transferase inhibitors
 INVENTOR(S): Casara, Patrick; Le Diguarher, Thierry; Dorey, Gilbert; Hickman, John; Pierre, Alain; Tucker, Gordon; Guilbaud, Nicolas; Ortuno, Jean-Claude; Fauchere, Jean-Luc
 PATENT ASSIGNEE(S): Les Laboratoires Servier, Fr.
 SOURCE: PCT Int. Appl., 78 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: French
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002057223	A2	20020725	WO 2002-FR147	20020116
WO 2002057223	A3	20021128		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
FR 2819511	A1	20020719	FR 2001-638	20010118
PRIORITY APPLN. INFO.:			FR 2001-638	A 20010118
OTHER SOURCE(S):	MARPAT 137:125097			
GI				



AB Title compds. I [W = CO, CH₂; X = bond, alkylene, CO, S(O)_n, S(O)_nA1, COA1, A1S(O)_nA2, A1COA2; Y = (un)substituted aryl, heteroaryl, cycloalkyl, heterocyclalkyl; T = NR1, NR1CO; V = H, (un)substituted aryl, heteroaryl; A1, A2 = alkylene; A3 = (CR₂R₃)_p; R1-R3 = H, (un)substituted alkyl, aryl, heteroaryl, aralkyl, heteroaralkyl; n = 0-2; p = 0-4] were prepared for use as farnesyl transferase inhibitors in the treatment of cancers, neurofibromatosis type 1, and restenosis after angioplasty or vascular surgery. Thus, (S)-3-amino-1-benzyl-2-azepanone was prepared from L-lysine in 4 steps and treated with 1-(4-cyanobenzyl)-1H-imidazole-5-carboxaldehyde, obtained by treating HOCH₂COCH₂OH with PhCH₂NH₂ and KSCN and oxidation of the resulting alc., to give the title compound II.

ED Entered STN: 26 Jul 2002

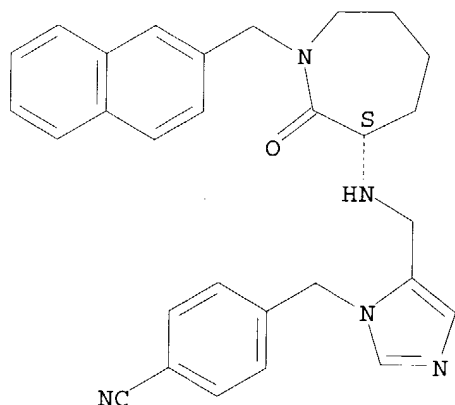
IT **443920-60-3P 443920-61-4P**

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(novel azepanes as farnesyl transferase inhibitors)

RN 443920-60-3 HCAPLUS

CN Benzonitrile, 4-[[5-[[[(3S)-hexahydro-1-(2-naphthalenylmethyl)-2-oxo-1H-azepin-3-yl]amino]methyl]-1H-imidazol-1-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 443920-61-4 HCAPLUS

CN Benzonitrile, 4-[[5-[[[(3S)-hexahydro-1-(2-naphthalenylmethyl)-2-oxo-1H-

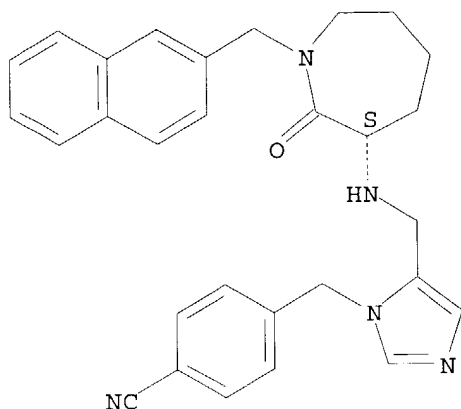
azepin-3-yl]amino]methyl]-1H-imidazol-1-yl]methyl]-, (2E)-2-butenedioate
(5:7) (9CI) (CA INDEX NAME)

CM 1

CRN 443920-60-3

CMF C29 H29 N5 O

Absolute stereochemistry.

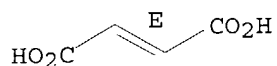


CM 2

CRN 110-17-8

CMF C4 H4 O4

Double bond geometry as shown.



L95 ANSWER 4 OF 30 HCAPLUS COPYRIGHT 2004 ACS on STN DUPLICATE 4
 ACCESSION NUMBER: 2002:571997 HCAPLUS
 DOCUMENT NUMBER: 137:169533
 TITLE: Preparation of microbiocidal N-phenyl-N-[4-(4-pyridyl)-pyrimidin-2-yl]amines
 INVENTOR(S): Eberle, Martin; Ziegler, Hugo; Cederbaum, Fredrik; Ackermann, Peter
 PATENT ASSIGNEE(S): Syngenta Participations A.-G., Switz.
 SOURCE: PCT Int. Appl., 50 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002053560	A1	20020711	WO 2001-XA2821	20011220
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS,				

LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PH, PL, PT, RO,
 RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ,
 VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,
 CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,
 BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
 WO 2002053560 A1 20020711 WO 2001-IB2821 20011220
 W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
 CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GH, GM,
 HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS,
 LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT,
 RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US,
 UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,
 CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,
 BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
 PRIORITY APPLN. INFO.: GB 2001-102 A 20010103
 WO 2001-IB2821 W 20011220
 GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. [I; m + p = 0-3; n, q = 0-1, and m + p + q = 1-4; R1 = H, halo, alkoxy, haloalkyl, haloalkoxy, alkyl; R2 = H, alkyl, haloalkyl, alkoxy; R2a = H, alkyl, alkenyl, alkynyl; R3-R6 = H, alkyl, haloalkyl, hydroxyalkyl, alkoxyalkyl, or the ring members CR3R4 or CR5R6 or CR2R2a = CO, CS; X = CO, CS, SO, SO2; Y = O, S, CO, CH2, etc.; R7 = H, alkyl, alkenyl, etc.], useful in controlling or preventing the infestation of plants by phytopathogenic microorganisms, especially fungi, were prepared

Thus, treating 2-{4-[2-(3-chlorophenylamino)pyrimidin-4-yl]pyridin-2-ylamino}ethanol with phosgene afforded II which showed over 70% control against Pyrenophora teres on barley. This is part II of I-II series.

ED Entered STN: 02 Aug 2002

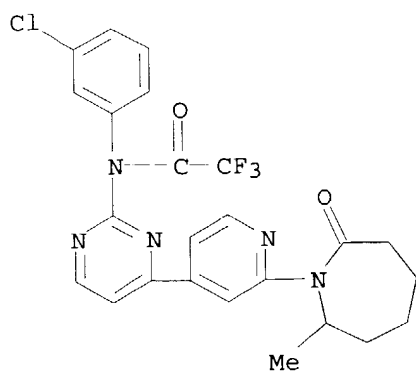
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 448277-11-0P 448277-14-3P 448277-15-4P
 448280-06-6P 448280-09-9P 448280-10-2P
 448283-17-8P 448283-20-3P 448283-21-4P
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 448289-56-3P 448289-59-6P 448289-60-9P
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RL: AGR (Agricultural use); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of microbiocidal N-phenyl-N-[4-(4-pyridyl)-pyrimidin-2-yl]amines)

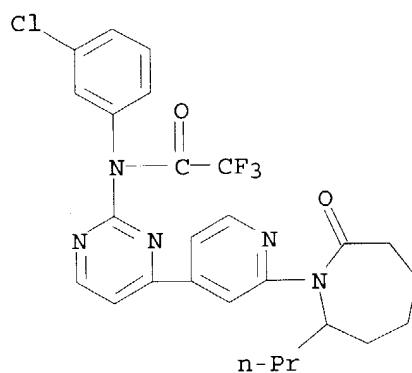
RN 448267-86-5 HCAPLUS

CN Acetamide, N-(3-chlorophenyl)-2,2,2-trifluoro-N-[4-[2-(hexahydro-2-methyl-7-oxo-1H-azepin-1-yl)-4-pyridinyl]-2-pyrimidinyl]- (9CI) (CA INDEX NAME)



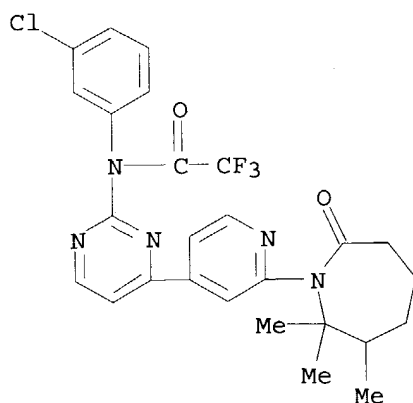
RN 448267-89-8 HCAPLUS

CN Acetamide, N-(3-chlorophenyl)-2,2,2-trifluoro-N-[4-[2-(hexahydro-2-oxo-7-propyl-1H-azepin-1-yl)-4-pyridinyl]-2-pyrimidinyl]- (9CI) (CA INDEX NAME)



RN 448267-90-1 HCAPLUS

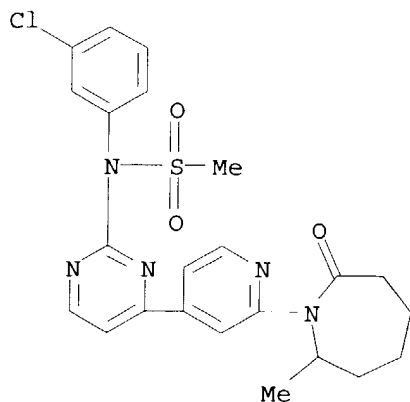
CN Acetamide, N-(3-chlorophenyl)-2,2,2-trifluoro-N-[4-[2-(hexahydro-2,2,3-trimethyl-7-oxo-1H-azepin-1-yl)-4-pyridinyl]-2-pyrimidinyl]- (9CI) (CA INDEX NAME)



RN 448270-89-1 HCAPLUS

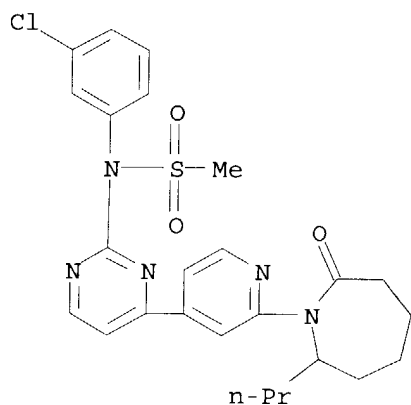
CN Methanesulfonamide, N-(3-chlorophenyl)-N-[4-[2-(hexahydro-2-methyl-7-oxo-

1H-azepin-1-yl)-4-pyridinyl]-2-pyrimidinyl]- (9CI) (CA INDEX NAME)



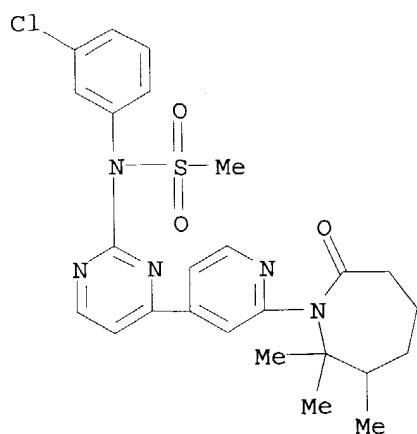
RN 448270-92-6 HCAPLUS

CN Methanesulfonamide, N-(3-chlorophenyl)-N-[4-[2-(hexahydro-2-oxo-7-propyl-1H-azepin-1-yl)-4-pyridinyl]-2-pyrimidinyl]- (9CI) (CA INDEX NAME)

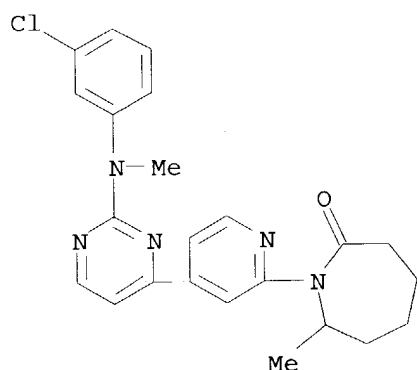


RN 448270-93-7 HCAPLUS

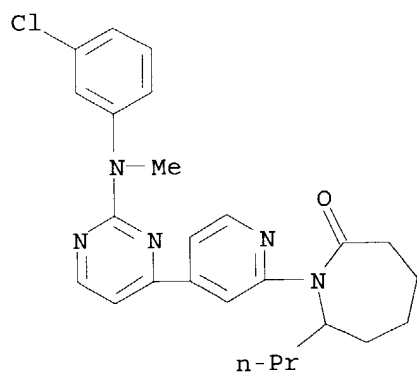
CN Methanesulfonamide, N-(3-chlorophenyl)-N-[4-[2-(hexahydro-2,2,3-trimethyl-7-oxo-1H-azepin-1-yl)-4-pyridinyl]-2-pyrimidinyl]- (9CI) (CA INDEX NAME)



RN 448274-18-8 HCAPLUS
 CN 2H-Azepin-2-one, 1-[4-[2-[(3-chlorophenyl)methylamino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-7-methyl- (9CI) (CA INDEX NAME)

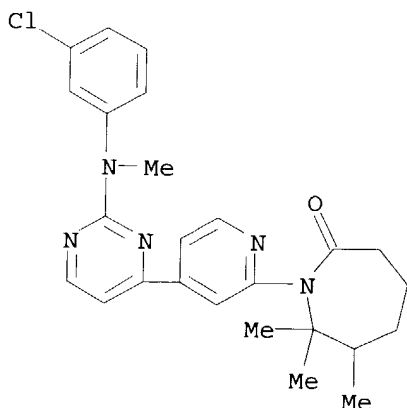


RN 448274-21-3 HCAPLUS
 CN 2H-Azepin-2-one, 1-[4-[2-[(3-chlorophenyl)methylamino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-7-propyl- (9CI) (CA INDEX NAME)



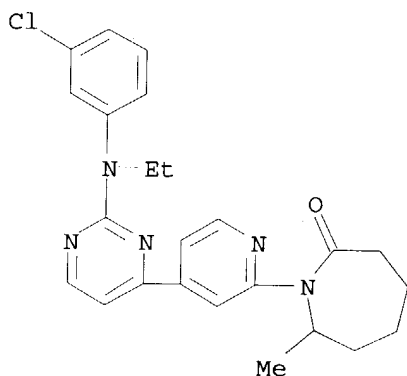
RN 448274-22-4 HCAPLUS
 CN 2H-Azepin-2-one, 1-[4-[2-[(3-chlorophenyl)methylamino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-7-n-propyl- (9CI) (CA INDEX NAME)

pyridinyl]hexahydro-6,7,7-trimethyl- (9CI) (CA INDEX NAME)



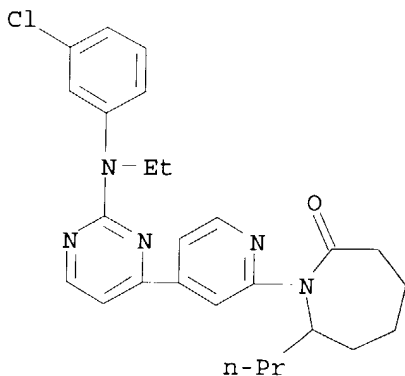
RN 448277-11-0 HCAPLUS

CN 2H-Azepin-2-one, 1-[4-[2-[(3-chlorophenyl)ethylamino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-7-methyl- (9CI) (CA INDEX NAME)



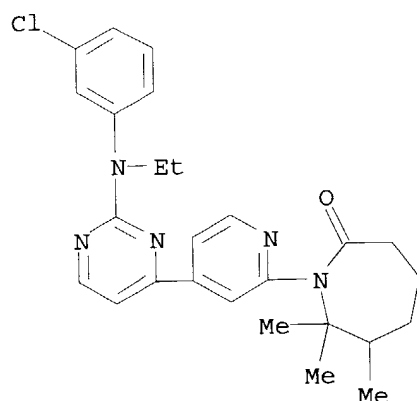
RN 448277-14-3 HCAPLUS

CN 2H-Azepin-2-one, 1-[4-[2-[(3-chlorophenyl)ethylamino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-7-propyl- (9CI) (CA INDEX NAME)

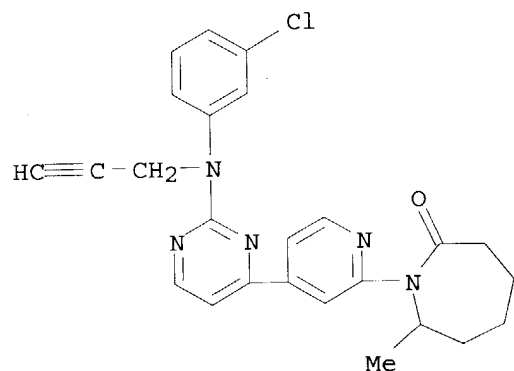


RN 448277-15-4 HCAPLUS

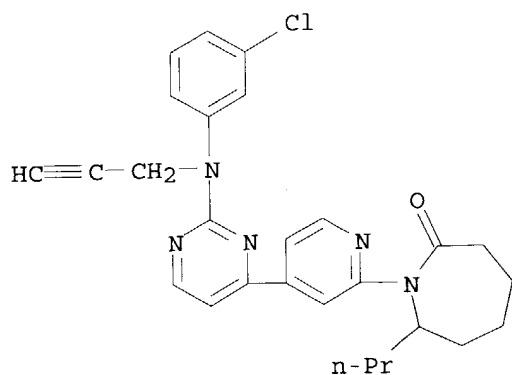
CN 2H-Azepin-2-one, 1-[4-[2-[(3-chlorophenyl)ethylamino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-6,7,7-trimethyl- (9CI) (CA INDEX NAME)



RN 448280-06-6 HCAPLUS
CN 2H-Azepin-2-one, 1-[4-[2-[(3-chlorophenyl)-2-propynylamino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-7-methyl- (9CI) (CA INDEX NAME)

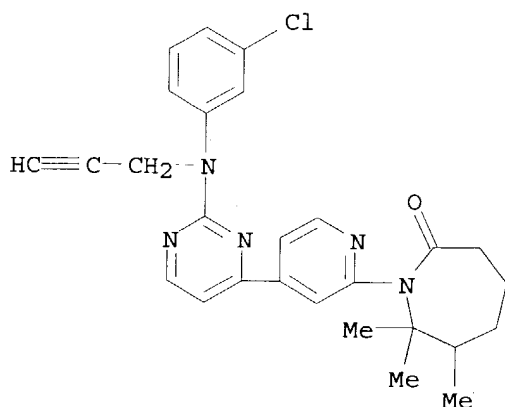


RN 448280-09-9 HCAPLUS
CN 2H-Azepin-2-one, 1-[4-[2-[(3-chlorophenyl)-2-propynylamino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-7-propyl- (9CI) (CA INDEX NAME)



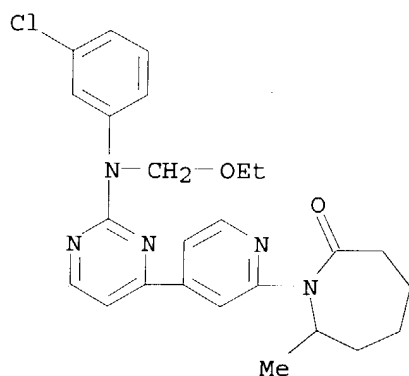
RN 448280-10-2 HCAPLUS

CN 2H-Azepin-2-one, 1-[4-[2-[(3-chlorophenyl)-2-propynylamino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-6,7,7-trimethyl- (9CI) (CA INDEX NAME)



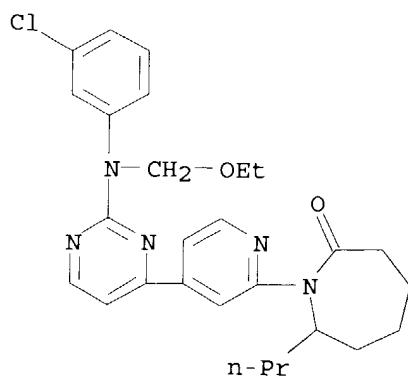
RN 448283-17-8 HCAPLUS

CN 2H-Azepin-2-one, 1-[4-[2-[(3-chlorophenyl) (ethoxymethyl) amino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-7-methyl- (9CI) (CA INDEX NAME)

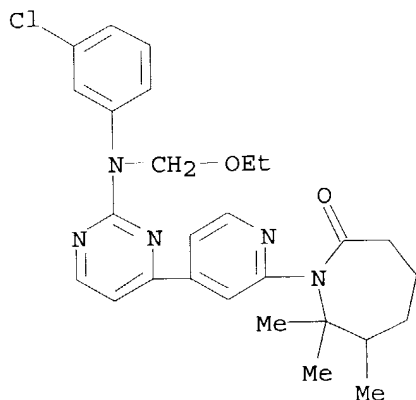


RN 448283-20-3 HCAPLUS

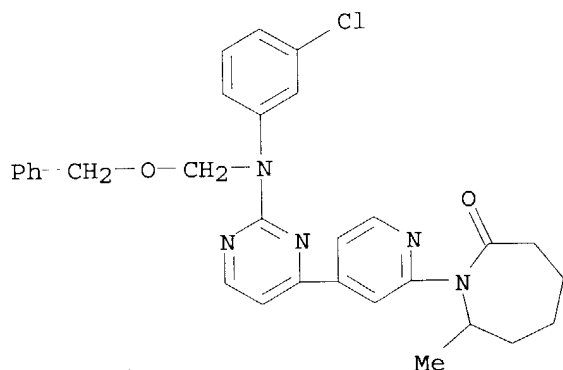
CN 2H-Azepin-2-one, 1-[4-[2-[(3-chlorophenyl) (ethoxymethyl) amino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-7-propyl- (9CI) (CA INDEX NAME)



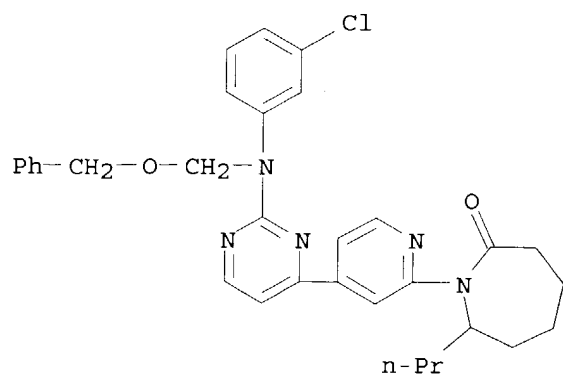
RN 448283-21-4 HCAPLUS
 CN 2H-Azepin-2-one, 1-[4-[2-[(3-chlorophenyl)(ethoxymethyl)amino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-6,7,7-trimethyl- (9CI) (CA INDEX NAME)



RN 448286-23-5 HCAPLUS
 CN 2H-Azepin-2-one, 1-[4-[2-[(3-chlorophenyl)[(phenylmethoxy)methyl]amino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-7-methyl- (9CI) (CA INDEX NAME)

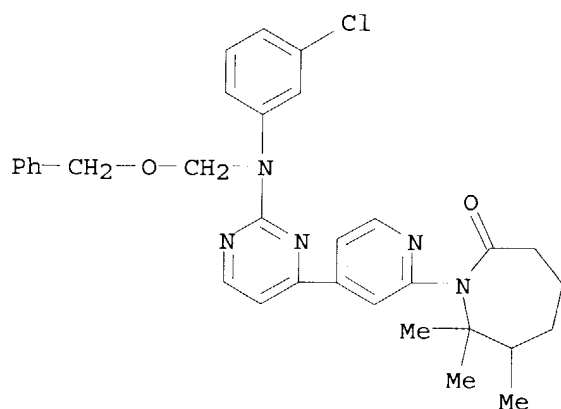


RN 448286-26-8 HCAPLUS
 CN 2H-Azepin-2-one, 1-[4-[2-[(3-chlorophenyl)[(phenylmethoxy)methyl]amino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-7-propyl- (9CI) (CA INDEX NAME)



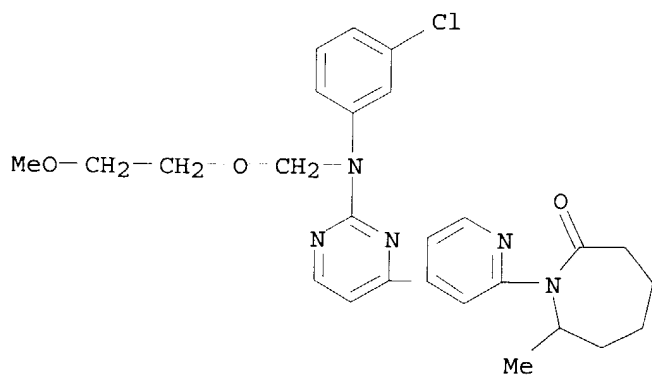
RN 448286-27-9 HCAPLUS

CN 2H-Azepin-2-one, 1-[4-[2-[(3-chlorophenyl)[(phenylmethoxy)methyl]amino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-6,7,7-trimethyl- (9CI) (CA INDEX NAME)



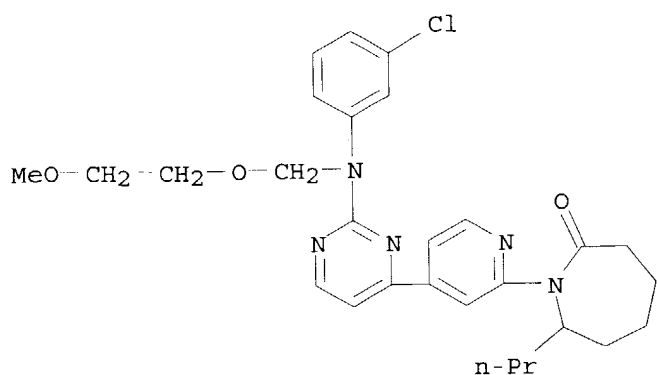
RN 448289-56-3 HCAPLUS

CN 2H-Azepin-2-one, 1-[4-[2-[(3-chlorophenyl)[(2-methoxyethoxy)methyl]amino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-7-methyl- (9CI) (CA INDEX NAME)

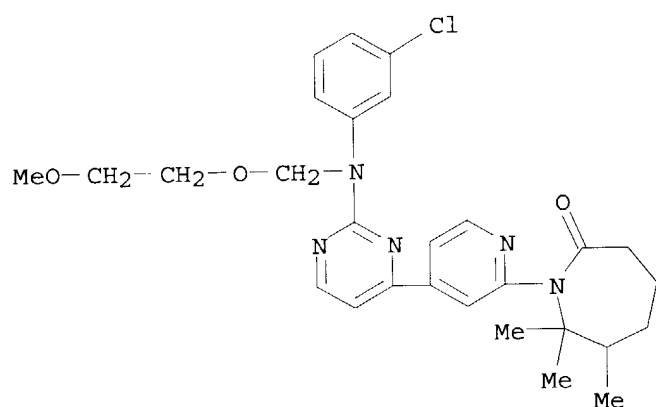


RN 448289-59-6 HCAPLUS

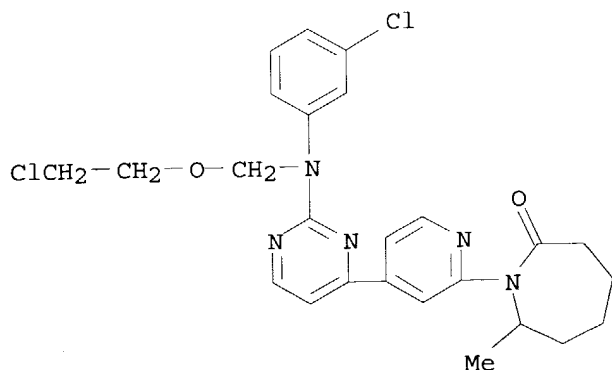
CN 2H-Azepin-2-one, 1-[4-[2-[(3-chlorophenyl)[(2-methoxyethoxy)methyl]amino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-7-propyl- (9CI) (CA INDEX NAME)



RN 448289-60-9 HCAPLUS
 CN 2H-Azepin-2-one, 1-[4-[2-[(3-chlorophenyl)[(2-methoxyethoxy)methyl]amino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-6,7,7-trimethyl- (9CI) (CA INDEX NAME)

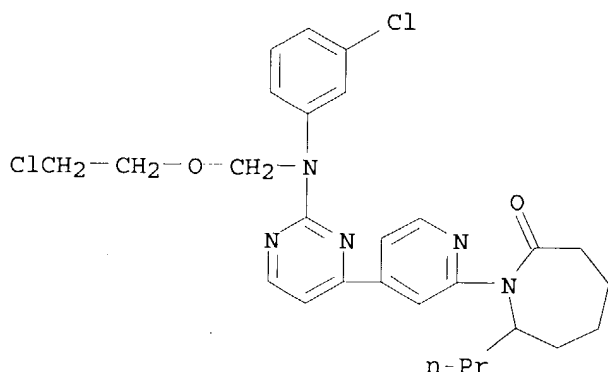


RN 448292-72-6 HCAPLUS
 CN 2H-Azepin-2-one, 1-[4-[2-[[[(2-chloroethoxy)methyl](3-chlorophenyl)amino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-7-methyl- (9CI) (CA INDEX NAME)



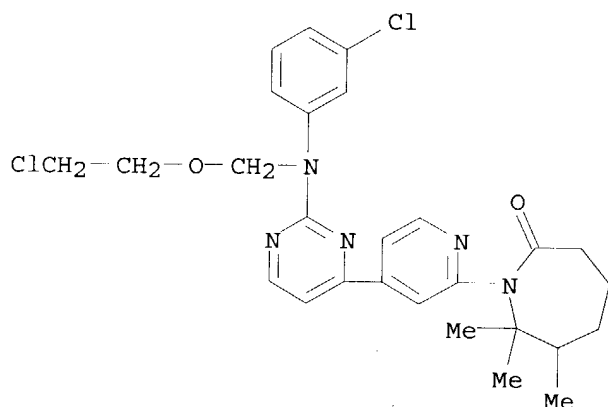
RN 448292-75-9 HCAPLUS

CN 2H-Azepin-2-one, 1-[4-[2-[[2-(chloroethoxy)methyl](3-chlorophenyl)amino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-7-propyl- (9CI) (CA INDEX NAME)



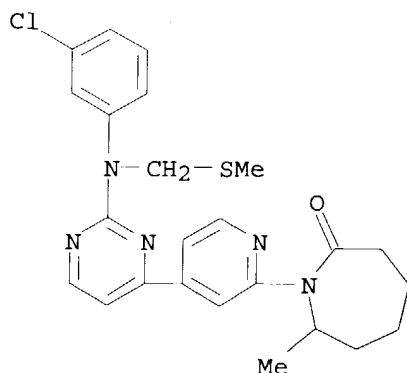
RN 448292-76-0 HCAPLUS

CN 2H-Azepin-2-one, 1-[4-[2-[[2-(chloroethoxy)methyl](3-chlorophenyl)amino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-6,7,7-trimethyl- (9CI) (CA INDEX NAME)

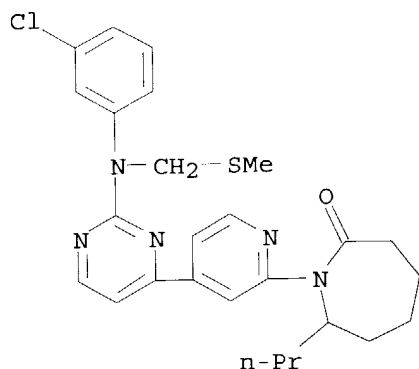


RN 448296-01-3 HCAPLUS

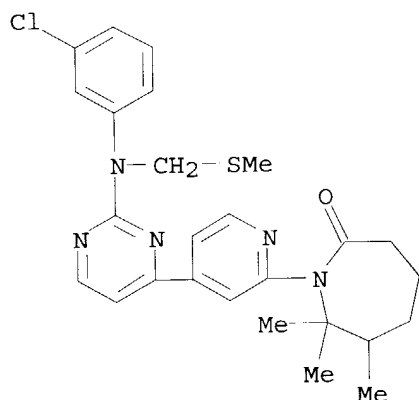
CN 2H-Azepin-2-one, 1-[4-[2-[(3-chlorophenyl)[(methylthio)methyl]amino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-7-methyl- (9CI) (CA INDEX NAME)



RN 448296-04-6 HCAPLUS
CN 2H-Azepin-2-one, 1-[4-[2-[(3-chlorophenyl)[(methylthio)methyl]amino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-7-propyl- (9CI) (CA INDEX NAME)



RN 448296-05-7 HCAPLUS
CN 2H-Azepin-2-one, 1-[4-[2-[(3-chlorophenyl)[(methylthio)methyl]amino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-6,7,7-trimethyl- (9CI) (CA INDEX NAME)



L95 ANSWER 5 OF 30 HCAPLUS COPYRIGHT 2004 ACS on STN DUPLICATE 5
ACCESSION NUMBER: 2002:103518 HCAPLUS
DOCUMENT NUMBER: 136:151180
TITLE: Preparation of caprolactam compounds and their use as inhibitors of serine proteases
INVENTOR(S): Bisacchi, Gregory S.; Seiler, Steven M.; Lawrence, R. Michael; Sutton, James C., Jr.; Slusarchyk, William A.; Zhao, Guohua
PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
SOURCE: U.S., 101 pp., Cont.-in-part of U.S. Ser. No. 478,632.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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US 6344450	B1	20020205	US 2000-633751	20000807
CA 2418995	AA	20020214	CA 2001-2418995	20010720
WO 2002012196	A2	20020214	WO 2001-US22829	20010720
WO 2002012196	A3	20030116		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

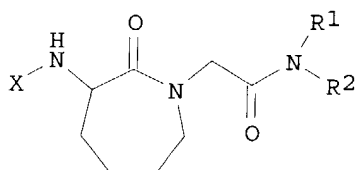
AU 2001080642	A5	20020218	AU 2001-80642	20010720
EP 1309609	A2	20030514	EP 2001-959048	20010720

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

JP 2004521071	T2	20040715	JP 2002-518174	20010720
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PRIORITY APPLN. INFO.: US 1999-119374P P 19990209
US 2000-478632 A2 20000106
US 2000-633751 A 20000807
WO 2001-US22829 W 20010720

OTHER SOURCE(S): MARPAT 136:151180
GI



I

AB Caprolactam (azepan-2-one) derivs. [I; R1, R2 = H, each (un)substituted alkyl, alkenyl, alkynyl, aryl, aminoalkylaryl, aminocycloalkylalkyl, aminoalkyl, aminoalkylcycloalkyl, heteroaryl, arylalkyl, heteroarylalkyl, cycloalkyl, cycloalkylalkyl, polycycloalkyl, polycycloalkylalkyl, cycloalkenyl, cycloheteroalkyl, cycloalkenylalkyl, polycycloalkenyl, or polycycloalkenylalkyl, or R1 and R2 can be taken with the nitrogen to which they are attached to form a cycloheteroalkyl ring; X = R4C(:Y), R3SO2 (wherein R3 is selected from optionally substituted alkyl, alkenyl, alkynyl, aryl, heteroaryl, arylalkyl, heteroarylalkyl, cycloalkyl, cycloalkylalkyl, polycycloalkyl, polycycloalkylalkyl, etc.; Y = O, S; R4 = R5R6N, R7O, R8; wherein R5, R6 = each optionally substituted alkyl, alkenyl, alkynyl, aryl, heteroaryl, arylalkyl, heteroarylalkyl, cycloalkyl, cycloalkylalkyl, polycycloalkyl, etc., or R5 and R6 can be taken with the nitrogen to which they are attached to form an optionally substituted cycloheteroalkyl ring; R7, R8 = each optionally substituted alkyl, alkenyl, alkynyl, aryl, heteroaryl, arylalkyl, heteroarylalkyl, cycloalkyl, cycloalkylalkyl, polycycloalkyl, polycycloalkylalkyl, cycloalkenyl, etc.)] are prepared These compds. are inhibitors of factor Xa and tryptase (no data) and thus are useful as anticoagulants and in treating asthma, resp. Methods for treating (1) cardiovascular diseases associated with thrombosis, (2) thrombosis, coronary artery disease or cerebrovascular disease, associated with thrombosis, and (3) inflammation, asthma, or allergic rhinitis are also provided. The above cardiovascular diseases are atherosclerotic plaques, venous or arterial thrombosis, coagulation syndromes, ischemia and angina (stable and unstable), deep

vein thrombosis (DVT), disseminated intravascular coagulopathy, Kasabach-Merritt syndrome, pulmonary embolism, myocardial infarction, cerebral infarction, cerebral thrombosis, atrial fibrillation, cerebral embolism, thromboembolic complications of surgery, peripheral arterial occlusion, or restenosis following arterial injury induced by endogenous or exogenous events. A method for treating inflammatory bowel disease, psoriasis, conjunctivitis, atopic dermatitis, rheumatoid arthritis, osteoarthritis, chronic inflammatory joint disease, diseases of joint cartilage destruction, allergic rhinitis myocardial infarction, stroke, angina, treating or preventing diabetic retinopathy, fibrosis, scleroderma, pulmonary fibrosis, liver cirrhosis, myocardial fibrosis, neurofibromas, and hypertrophic scars is also provided. Thus, in an automated solution synthesis, a stock solution of 7 mg 4-[2-(methylamino)ethyl]pyridine in THF (300 μ L), a stock solution of 8 mg diisopropylcarbodiimide in CH_2Cl_2 (300 μ L), and a stock solution of 12 mg 7-aza-1-hydroxybenzotriazole in DMF (300 μ L), and a stock solution of 2-[(3S)-3-[N'-(3-methylphenyl)ureido]-2-oxoazepan-2-yl]acetic acid (preparation given) in CH_2Cl_2 , were added via a liquid handler to a 16 mm + 100 mm tube and mixed in an orbital shaker for 72 h to give 2-[(3S)-3-[N'-(3-methylphenyl)ureido]-2-oxoazepan-2-yl]-N-methyl-N-[2-(4-pyridyl)ethyl]acetamide.

ED Entered STN: 07 Feb 2002

IT **288269-39-6P**

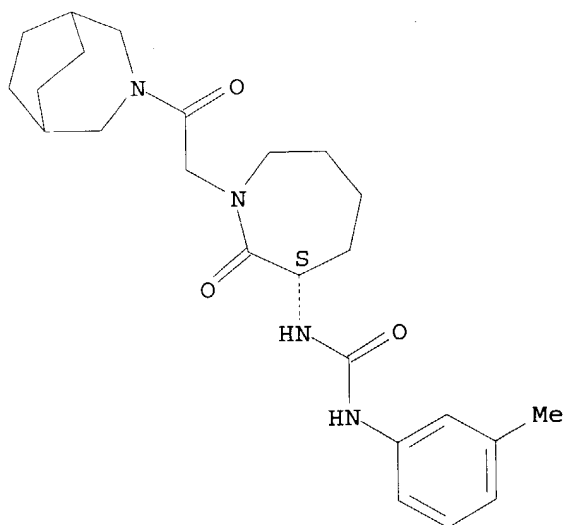
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of lactam compds. as inhibitors of serine proteases and factor Xa and anticoagulants for treating thrombosis-associated diseases, asthma, inflammation, or allergic rhinitis.)

RN 288269-39-6 HCAPLUS

CN 3-Azabicyclo[3.2.2]nonane, 3-[[[(3S)-hexahydro-3-[[[(3-methylphenyl)amino]carbonyl]amino]-2-oxo-1H-azepin-1-yl]acetyl]- (9CI)
(CA INDEX NAME)

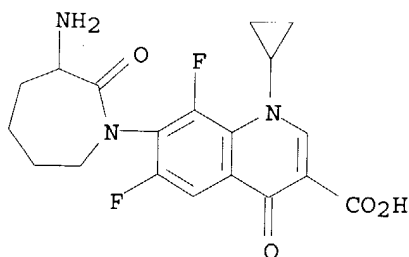
Absolute stereochemistry.



REFERENCE COUNT:

29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L95 ANSWER 6 OF 30 HCAPLUS COPYRIGHT 2004 ACS on STN DUPLICATE 6
 ACCESSION NUMBER: 1995:38543 HCAPLUS
 DOCUMENT NUMBER: 122:156098
 TITLE: In vitro anti-Mycobacterium avium activities of quinolones: predicted active structures and mechanistic considerations
 AUTHOR(S): Klopman, Gilles; Li, Ju-Yun; Wang, Shaomeng; Pearson, Anthony J.; Chang, Kieyoung; Jacobs, Michael R.; Bajaksouzian, Saralee; Ellner, Jerrold J.
 CORPORATE SOURCE: Chem. Dept., Case Western Res. Univ., Cleveland, OH, 44106, USA
 SOURCE: Antimicrobial Agents and Chemotherapy (1994), 38(8), 1794-1802
 CODEN: AMACCO; ISSN: 0066-4804
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The relation between the structures of quinolones and their anti-M. avium activities has been previously derived by using the Multiple Computer-Automated Structure Evaluation program. A number of substructural constraints required to overcome the resistance of most of the strains have been identified. Nineteen new quinolones which qualify under these substructural requirements were identified by the program and subsequently tested. The substructural attributes identified by the program produced a successful a priori prediction of the anti-M. avium activities of the new quinolones. All 19 quinolones were active, and 4 of them are as active or better than ciprofloxacin. With these new quinolones, the updated multiple computer-automated structure evaluation program structure-activity relationship anal. has helped to uncover addnl. information about the nature of the substituents at the C5 and C7 positions needed for optimal inhibitory activity. A possible explanation of drug resistance based on the observation of suicide inactivation of bacterial cytochrome P 450 by the cyclopropylamine moiety has also been proposed and is discussed in this report. The view that the amount of the uncharged form present in a neutral pH solution plays a crucial role in the drug's penetration ability was confirmed.
 ED Entered STN: 08 Nov 1994
 IT 151895-29-3, PD 130426
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
 (anti-Mycobacterium activity of)
 RN 151895-29-3 HCAPLUS
 CN 3-Quinolonecarboxylic acid, 7-(3-amino-6,8-difluoro-1,4-dihydro-4-oxo-1H-cyclopropyl)-1-cyclopropyl-6,8-difluoro-1,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



L95 ANSWER 7 OF 30 HCAPLUS COPYRIGHT 2004 ACS on STN DUPLICATE 7
 ACCESSION NUMBER: 1995:2483 HCAPLUS
 DOCUMENT NUMBER: 123:164953

TITLE: Anti-mycobacterium avium activity of quinolones: in vitro activities. [Erratum to document cited in CA120:27300f]

AUTHOR(S): Klopman, Gilles; Wang, Shaomeng; Jacobs, Michael R.; Bajaksouzian, Saralee; Edmonds, Kay; Ellner, Jerrold J.

CORPORATE SOURCE: Chem. Dep., Case West. Reserve Univ., Cleveland, OH, 44106, USA

SOURCE: Antimicrobial Agents and Chemotherapy (1993), 37(12), 2766
CODEN: AMACCQ; ISSN: 0066-4804

DOCUMENT TYPE: Journal

LANGUAGE: English

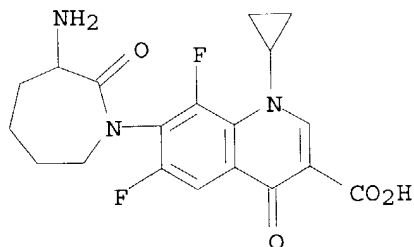
AB The errors were not reflected in the abstract or the index entries.

ED Entered STN: 08 Nov 1994

IT 151895-29-3
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(Mycobacterium avium sensitivity to (Erratum))

RN 151895-29-3 HCAPLUS

CN 3-Quinolonecarboxylic acid, 7-(3-amino-6,8-difluoro-1,4-dihydro-4-oxo-1H-azepin-1-yl)-1-cyclopropyl-6,8-difluoro-1,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



L95 ANSWER 8 OF 30 HCAPLUS COPYRIGHT 2004 ACS on STN DUPLICATE 8

ACCESSION NUMBER: 1994:27300 HCAPLUS

DOCUMENT NUMBER: 120:27300

TITLE: Anti-mycobacterium avium activity of quinolones: in vitro activities

AUTHOR(S): Klopman, Gilles; Wang, Shaomeng; Jacobs, Michael R.; Bajaksouzian, Saralee; Edmonds, Kay; Ellner, Jerrold J.

CORPORATE SOURCE: Chem. Dep., Case West. Reserve Univ., Cleveland, OH, 44106, USA

SOURCE: Antimicrobial Agents and Chemotherapy (1993), 37(9), 1799-806
CODEN: AMACCQ; ISSN: 0066-4804

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The MICs of 88 quinolones against 14 selected reference and clin. strains of Mycobacterium avium-M. intracellulare complex were determined Agents tested included ciprofloxacin, sparfloxacin (PD 131501), and 86 other exptl. quinolones. Test strains were selected to represent various susceptibilities to ciprofloxacin and other drug resistance profiles. MICs were determined by the microdilution method in 7HSF broth, with incubation for 14 days at 35°. The results showed 25 of the quinolones to be active against the strains, with MICs for 90% of the strains (MIC90s) of 2

to 32 µg/mL. Ten of these compds. had activities equivalent to or greater than that of ciprofloxacin. The most active compound was PD 125354, with an MIC₅₀ of 0.5 µg/mL and an MIC₉₀ of 2 µg/mL; comparable values for ciprofloxacin were 4 and 8 µg/mL, resp. The next most active compds., with MIC₉₀s of 4 µg/mL, were sparfloxacin (PD 131501), PD 123982, PD 135144, and PD 119421. MIC₉₀s of PD 131575, PD 126889, PD 122642, PD 139586, and PD 143289 were 8 µg/mL. Further evaluation of the most active agents is warranted, as is assessment of structure-activity relationships of active and inactive agents to elucidate the active portions of the compds. and to lead to the development of compds. with enhanced activity.

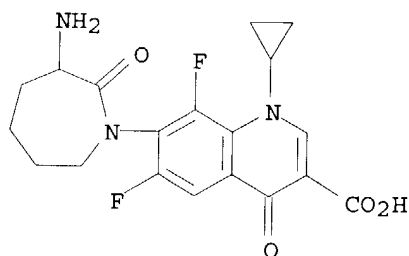
ED Entered STN: 22 Jan 1994

IT 151895-29-3

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(Mycobacterium avium sensitivity to)

RN 151895-29-3 HCAPLUS

CN 3-Quinolinecarboxylic acid, 7-(3-aminohexahydro-2-oxo-1H-azepin-1-yl)-1-cyclopropyl-6,8-difluoro-1,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



L95 ANSWER 9 OF 30 HCAPLUS COPYRIGHT 2004 ACS on STN DUPLICATE 9

ACCESSION NUMBER: 1992:530937 HCAPLUS

DOCUMENT NUMBER: 117:130937

TITLE: Derivatives of 1,2,3,4-tetrahydronaphthylamine endowed with nootropic activity and pharmaceutical compositions containing same

INVENTOR(S): Giannessi, Fabio; Ghirardi, Orlando; Misiti, Domenico; Tinti, Maria Ornella; Cozzolino, Roberto

PATENT ASSIGNEE(S): Sigma-Tau Industrie Farmaceutiche Riunite S.p.A., Italy

SOURCE: Eur. Pat. Appl., 15 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

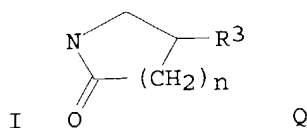
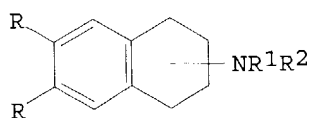
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 493346	A2	19920701	EP 1991-830574	19911219
EP 493346	A3	19920826		
EP 493346	B1	19950614		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, MC, NL, SE				
US 5192759	A	19930309	US 1991-809874	19911218
ES 2073725	T3	19950816	ES 1991-830574	19911219
JP 04275264	A2	19920930	JP 1991-338442	19911220
PRIORITY APPLN. INFO.:			IT 1990-48605	A 19901221

OTHER SOURCE(S):
GI

MARPAT 117:130937



AB The title compds. I [R = H, OMe; NR1R2 is at the 1- or 2-position; R1 = H; R2 = L-prolyl, optionally substituted, L-pyrroglutamyl, (pyrrolidin-2-on-1-yl)acetyl, 3-carboxy-2-hydroxypropyl; NR1R2 = Q (n = 1, 2, 3 and R3 = H, OH)] were prepared as nootropic agents. E.g., reaction of Z-L-proline and 1,2,3,4-tetrahydro-6,7-dimethoxy-2-naphthylamine in MeCN in the presence of EEDQ gave 85% product, which was hydrogenated in MeOH with 10% Pd/C at 40 psi for 2 h to give 71% N-(L-prolyl)-1,2,3,4-tetrahydro-6,7-dimethoxy-2-naphthylamine (II). Of the compds. prepared and tested, only II showed anti-amnesic activity, without toxicity, in scopolamine- and electroconvulsive shock-induced amnesia.

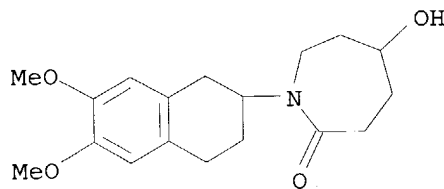
ED Entered STN: 04 Oct 1992

IT 143254-67-5P 143254-69-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

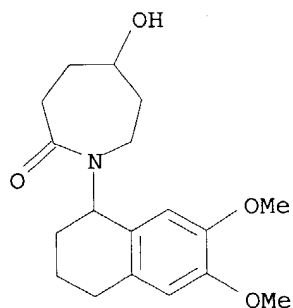
RN 143254-67-5 HCAPLUS

CN 2H-Azepin-2-one, hexahydro-5-hydroxy-1-(1,2,3,4-tetrahydro-6,7-dimethoxy-2-naphthalenyl)- (9CI) (CA INDEX NAME)



RN 143254-69-7 HCAPLUS

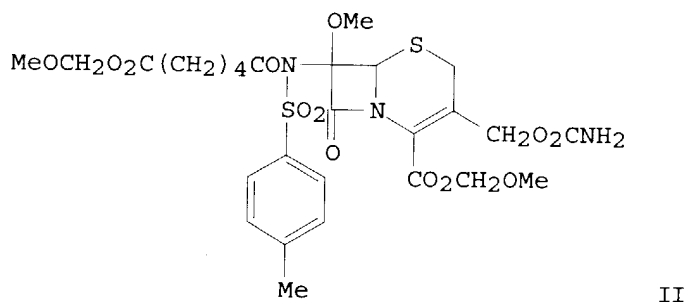
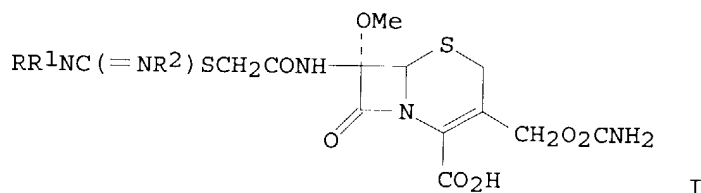
CN 2H-Azepin-2-one, hexahydro-5-hydroxy-1-(1,2,3,4-tetrahydro-6,7-dimethoxy-1-naphthalenyl)- (9CI) (CA INDEX NAME)



L95 ANSWER 10 OF 30 HCAPLUS COPYRIGHT 2004 ACS on STN DUPLICATE 10

ACCESSION NUMBER: 1979:87491 HCAPLUS
 DOCUMENT NUMBER: 90:87491
 TITLE: 7-(Amidinothio)acetamido-7-methoxycephalosporins
 INVENTOR(S): Czaja, Robert F.; Grabowski, Edward J. J.
 PATENT ASSIGNEE(S): Merck and Co., Inc., USA
 SOURCE: U.S., 3 pp.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4121041	A	19781017	US 1977-765477	19770204
PRIORITY APPLN. INFO.: GI			US 1977-765477	19770204



AB Cephalosporins I [R, R₁, R₂ = H, C1-5 alkyl, Ph; RR₁ = (CH₂)_n (n = 3-6)] were prepared by treating RR₁NCSNR₂H with a 7-chloro- or 7-bromoacetamidocephem. Thus, II treated with ClCH₂COCl gave the mono-Me ester which was saponified to give I (R - R₂ = H).

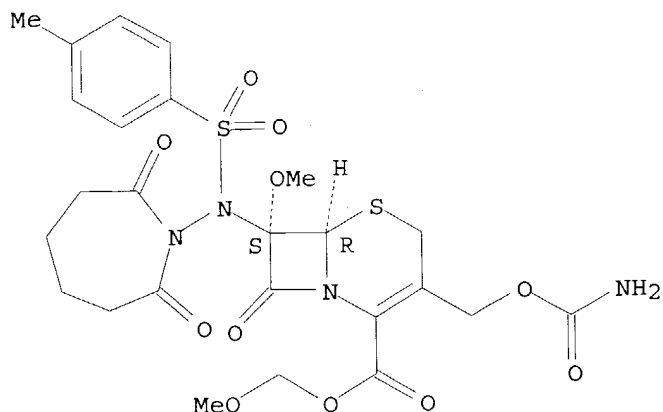
ED Entered STN: 12 May 1984

IT **69195-89-7**
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with chloroacetyl chloride)

RN 69195-89-7 HCAPLUS

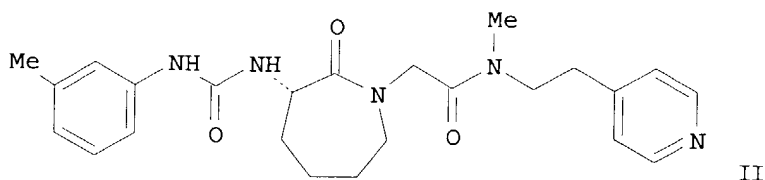
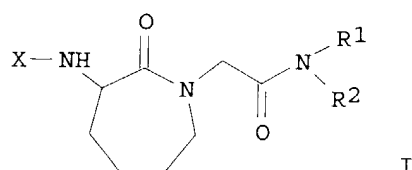
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
 3-[[aminocarbonyl]oxy]methyl]-7-[(hexahydro-2,7-dioxo-1H-azepin-1-yl)][(4-methylphenyl)sulfonyl]amino]-7-methoxy-8-oxo-, methoxymethyl ester,
 (6R-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L95 ANSWER 11 OF 30 HCAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 2000:573779 HCAPLUS
 DOCUMENT NUMBER: 133:177117
 TITLE: Preparation of lactam inhibitors of FXa
 INVENTOR(S): Bisacchi, Gregory S.; Seiler, Steven M.; Lawrence, R. Michael
 PATENT ASSIGNEE(S): Bristol-Myers Squibb Co., USA
 SOURCE: PCT Int. Appl., 58 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000047563	A1	20000817	WO 2000-US1859	20000127
W:	AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
CA 2361919	AA	20000817	CA 2000-2361919	20000127
EP 1175405	A1	20020130	EP 2000-904564	20000127
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO			
AU 756174	B2	20030109	AU 2000-26300	20000127
PRIORITY APPLN. INFO.:			US 1999-119374P	P 19990209
			WO 2000-US1859	W 20000127
OTHER SOURCE(S):	MARPAT 133:177117			
GI				



AB Lactam inhibitors of formula I [R1, R2 = alkyl, alkenyl, aryl, heteroaryl, cycloalkyl, etc.; R1R2 = cycloheteroalkyl; X = (substituted) CO, (substituted) CS, (substituted) SO2, etc.] are prepared. These compds. are inhibitors of Factor Xa and thus are useful as anticoagulants (no data). A method for treating cardiovascular diseases associated with thromboses is also provided. Thus, II was prepared from 3-tert-butoxycarbonylamino-hexahydro-2-azepinone, Et bromoacetate, m-tolylisocyanate and methylaminoethylpyridine.

ED Entered STN: 18 Aug 2000

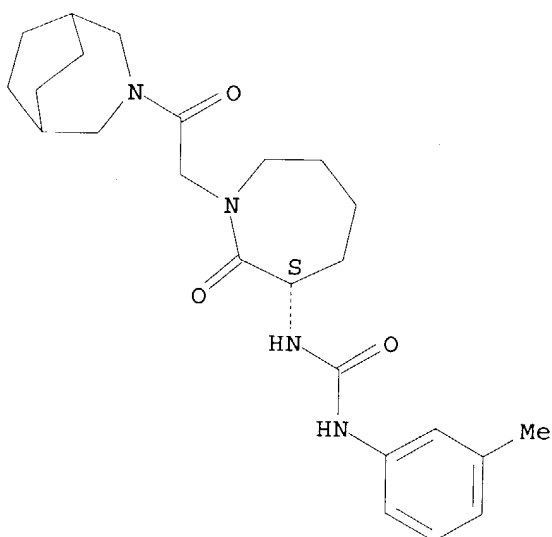
IT **288269-39-6P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of lactam inhibitors of Factor Xa)

RN 288269-39-6 HCAPLUS

CN 3-Azabicyclo[3.2.2]nonane, 3-[[[(3S)-hexahydro-3-[[[(3-methylphenyl)amino]carbonyl]amino]-2-oxo-1H-azepin-1-yl]acetyl]- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L95 ANSWER 12 OF 30 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2000:573666 HCAPLUS

DOCUMENT NUMBER: 133:164010

TITLE: Preparation of caprolactams, piperidinones, and pyrrolidinones as Factor Xa inhibitors in prevention or treatment of thromboses, coronary artery disease, or cerebrovascular disease in mammals

INVENTOR(S): Stein, Philip D.; Bisacchi, Gregory S.; Shi, Yan; O'Connor, Stephen P.; Li, Chi

PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA

SOURCE: PCT Int. Appl., 284 pp.

CODEN: PIXXD2

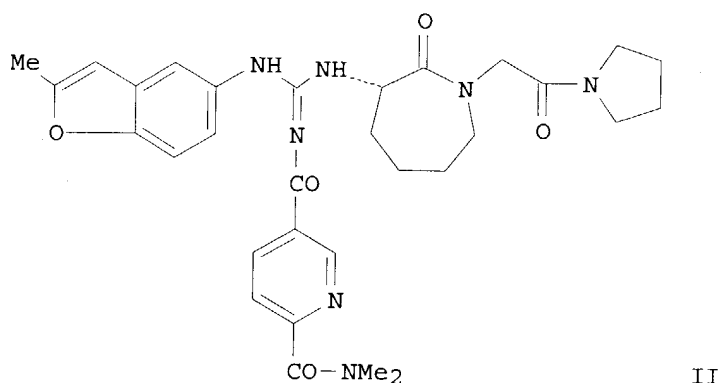
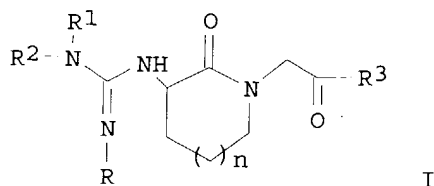
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000047207	A1	20000817	WO 2000-US2883	20000202
W:	AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
CA 2360305	AA	20000817	CA 2000-2360305	20000202
US 6297233	B1	20011002	US 2000-496571	20000202
EP 1156803	A1	20011128	EP 2000-914505	20000202
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO			
AU 760174	B2	20030508	AU 2000-35887	20000202
PRIORITY APPLN. INFO.:			US 1999-119372P	P 19990209
			US 1999-167428P	P 19991124
			WO 2000-US2883	W 20000202
OTHER SOURCE(S):	MARPAT 133:164010			
GI				



AB Title chiral compds. [I; R = CN, CONH₂, COOCH₂CH₃, COC₆H₅, SO₂NH₂, OCH₃, SO₂N(CH₃)₂, SO₂CH₃, arylsulfonyl, heterocyclosulfonyl, (un)substituted Ph, heterocyclyl, heterocycleocarbonyl, alkoxycarbonyl, arylaminocarbonyl; R₁ = H, arylalkyl; R₂ = alkyl, (un)substituted Ph, benzoheterocyclyl, cyclopentyl; R₃ = heterocyclylamino, heterocyclyl, alkoxy, cycloalkylamino, OH; n = 0, 1, 2] , pharmaceutically acceptable salts, and stereoisomers are pred. as Factor Xa inhibitors and are useful as anticoagulants (no data). A method for treating cardiovascular diseases associated with thromboses is also provided. Thus, the title compound II was prepared

ED Entered STN: 18 Aug 2000

IT 288077-09-8P 288077-32-7P 288077-40-7P
288081-29-8P 288081-35-6P 288081-83-4P
288082-97-3P

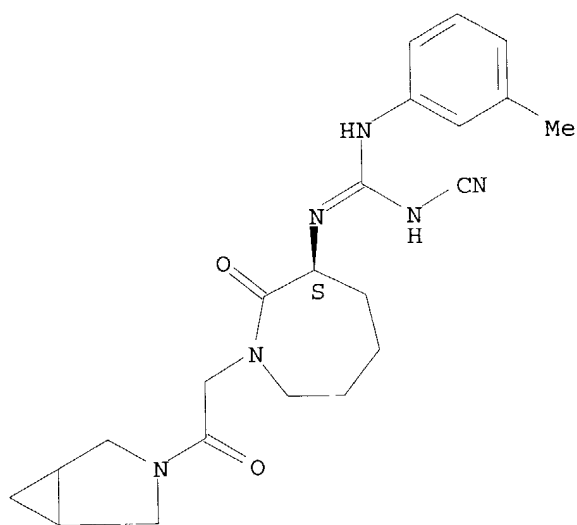
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of caprolactams as Factor Xa inhibitors in prevention or treatment of thromboses, coronary artery disease, or cerebrovascular disease in mammals)

RN 288077-09-8 HCAPLUS

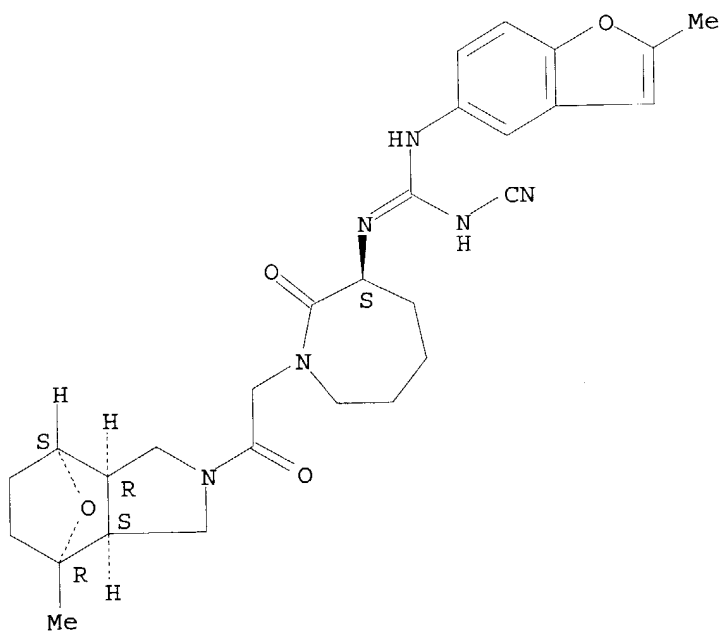
CN 3-Azabicyclo[3.1.0]hexane, 3-[[[(3S)-3-[[[(cyanoamino)[(3-methylphenyl)amino]methylene]amino]hexahydro-2-oxo-1H-azepin-1-yl]acetyl]]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



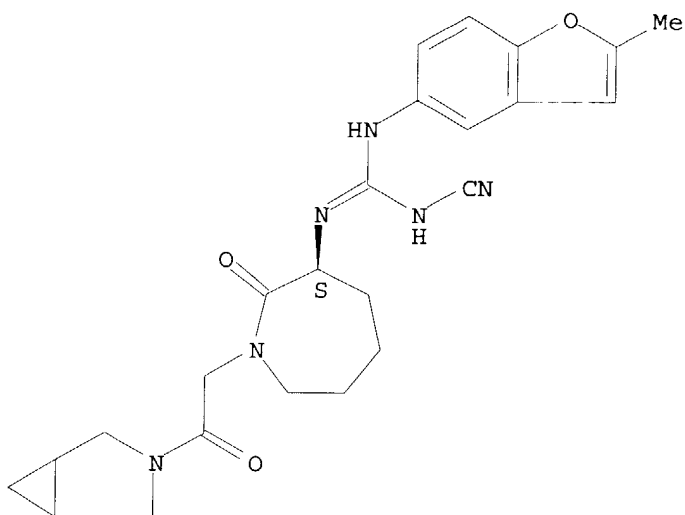
RN 288077-32-7 HCAPLUS
 CN 4,7-Epoxy-1H-isoindole, 2-[[[(3S)-3-[[[(cyanoamino)[(2-methyl-5-benzofuranyl)amino]methylene]amino]hexahydro-2-oxo-1H-azepin-3-yl]acetyl]octahydro-4-methyl-, (3aS,4R,7S,7aR)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 288077-40-7 HCAPLUS
 CN 3-Azabicyclo[3.1.0]hexane, 3-[[[(3S)-3-[[[(cyanoamino)[(2-methyl-5-benzofuranyl)amino]methylene]amino]hexahydro-2-oxo-1H-azepin-1-yl]acetyl]-(9CI) (CA INDEX NAME)

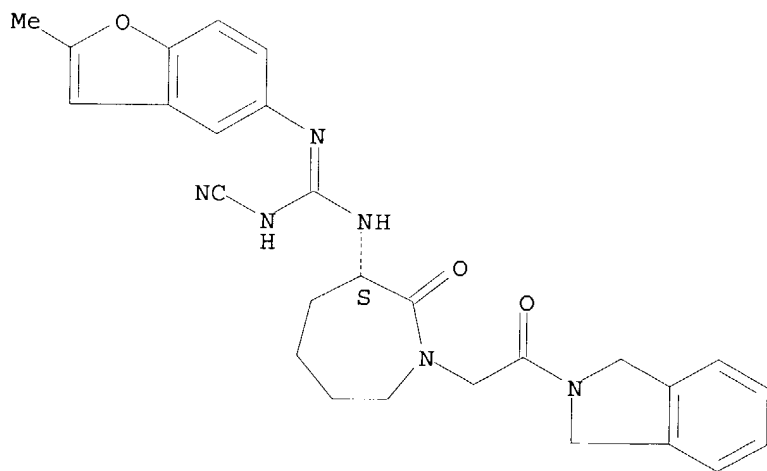
Absolute stereochemistry.



RN 288081-29-8 HCAPLUS

CN 1H-Isoindole, 2-[[[(3S)-3-[[[(cyanoamino)[(2-methyl-5-benzofuranyl)amino]methylene]amino]hexahydro-2-oxo-1H-azepin-1-yl]acetyl]-2,3-dihydro- (9CI) (CA INDEX NAME)

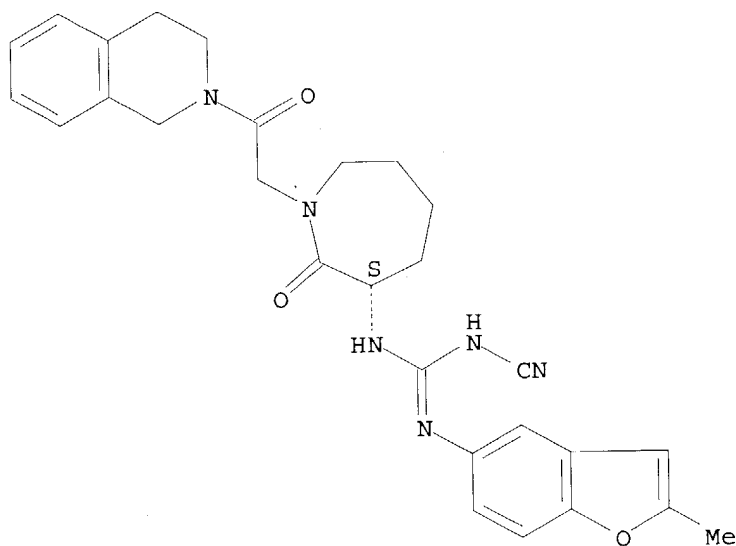
Absolute stereochemistry.



RN 288081-35-6 HCAPLUS

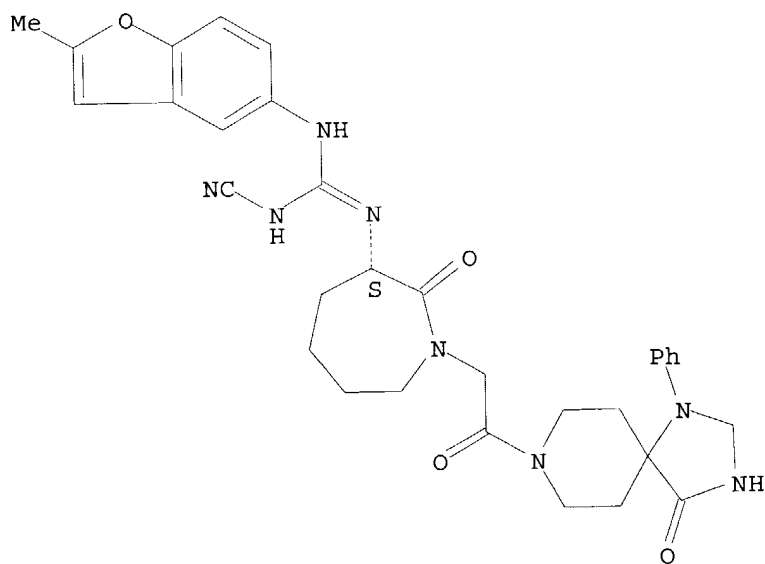
CN Isoquinoline, 2-[[[(3S)-3-[[[(cyanoamino)[(2-methyl-5-benzofuranyl)amino]methylene]amino]hexahydro-2-oxo-1H-azepin-1-yl]acetyl]-1,2,3,4-tetrahydro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



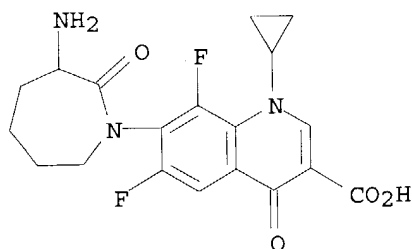
RN 288081-83-4 HCAPLUS
 CN 1,3,8-Triazaspiro[4.5]decan-4-one, 8-[[[(3S)-3-[[[(cyanoamino)[(2-methyl-5-benzofuranyl)amino]methylene]amino]hexahydro-2-oxo-1H-azepin-1-yl]acetyl]-1-phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 288082-97-3 HCAPLUS
 CN 3-Azabicyclo[3.1.0]hexane, 3-[[[3-[[[(cyanoamino)[(2-methyl-5-benzofuranyl)amino]methylene]amino]hexahydro-2-oxo-1H-azepin-1-yl]acetyl]-1-phenyl- (9CI) (CA INDEX NAME)

ACCESSION NUMBER: 1998:34271 HCAPLUS
DOCUMENT NUMBER: 128:212700
TITLE: Activity of new quinolones against intracellular Mycobacterium avium in human monocytes
AUTHOR(S): Venkataprasad, Nandagopal; Jacobs, Michael R.; Johnson, John L.; Klopman, Gilles; Ellner, Jerrold J.
CORPORATE SOURCE: Division of Infectious Diseases, Case Western Reserve University, OH, 44106, USA
SOURCE: Journal of Antimicrobial Chemotherapy (1997), 40(6), 841-845
CODEN: JACHDX; ISSN: 0305-7453
PUBLISHER: Oxford University Press
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The ability to inhibit the in-vitro growth of mycobacteria within human monocytes is a useful screening assay for novel chemotherapeutic agents. In this study the MICs of a panel of new quinolones were determined by the broth microdilution method for two strains of Mycobacterium avium. Sixteen such compds. with MIC90s ranging from 2 to >32 mg/L were subsequently selected for the 7 day monocyte assay using ciprofloxacin for comparison. The degree of inhibition of intracellular growth correlated with the MICs. PD 139586, PD 143289, PD 135144, PD 119421 and PD 131575 were the most active new agents with activities superior to those of ciprofloxacin and sparfloxacin.
ED Entered STN: 21 Jan 1998
IT 151895-29-3, PD 130426
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(activity of new quinolones against intracellular Mycobacterium avium in human monocytes)
RN 151895-29-3 HCAPLUS
CN 3-Quinolonecarboxylic acid, 7-(3-aminohexahydro-2-oxo-1H-azepin-1-yl)-1-cyclopropyl-6,8-difluoro-1,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L95 ANSWER 15 OF 30 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1994:288561 HCAPLUS
DOCUMENT NUMBER: 120:288561
TITLE: CO2 transfer by metal phenoxides: N-methyl-ε-caprolactam/sodium phenoxide as a selective reagent for carboxylation reactions
AUTHOR(S): Walther, D.; Ritter, U.; Gessler, S.; Sieler, J.; Kunert, M.
CORPORATE SOURCE: Inst. Anorg. Anal. Chem., Friedrich-Schiller-Univ., Jena, Germany

SOURCE: Zeitschrift fuer Anorganische und Allgemeine Chemie
(1994), 620(1), 101-6

CODEN: ZAACAB; ISSN: 0044-2313

DOCUMENT TYPE: Journal

LANGUAGE: German

AB Carboxylation reactions of acetone and other substrates with active C-H bonds can be carried out selectively by complexes of NaOPh with N-methyl-ε-caprolactam (NMC) and CO₂. With acetone 3-keto-glutaric acid is formed in 85% yield upon hydrolysis. X-ray structural anal. of [(NMC)Na(OPh)]₄ shows that Na⁺ and O⁻ ions of the phenoxide occupy the positions of a cube. NMC acts as monodentate ligand, the O atoms of the phenoxide are tridentate bridging ligands. The Li compound has a similar structure. The complex dissolved in NMC takes up 0.5 mol CO₂ per mol Na which at room temperature and normal pressure is transferred to acetone.

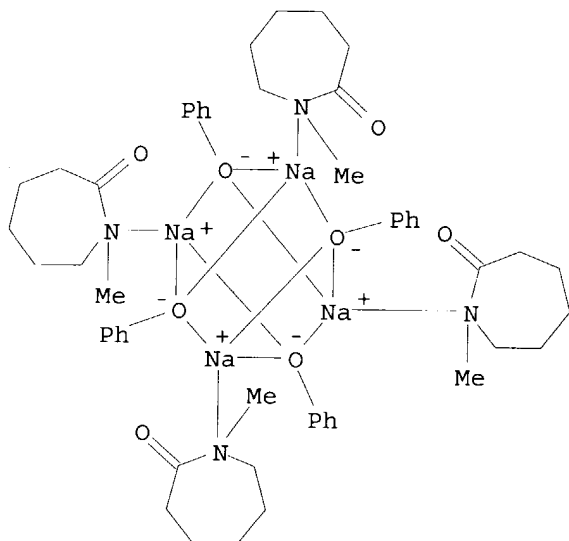
ED Entered STN: 28 May 1994

IT 154935-77-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal structure and transfer agent in carboxylation of acetone)

RN 154935-77-0 HCAPLUS

CN Sodium, tetrakis(hexahydro-1-methyl-2H-azepin-2-one-N1)tetra-μ₃-phenoxytetra- (9CI) (CA INDEX NAME)

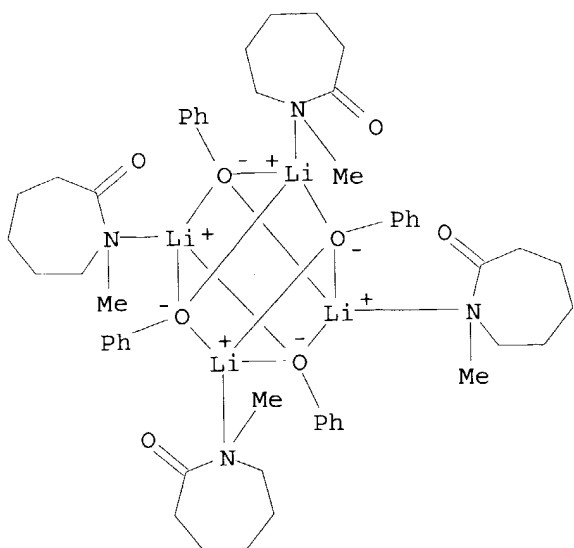


IT 154935-78-1P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal structure of)

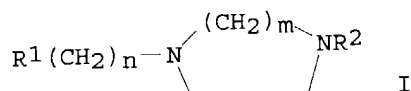
RN 154935-78-1 HCAPLUS

CN Lithium, tetrakis(hexahydro-1-methyl-2H-azepin-2-one-N1)tetra-μ₃-phenoxytetra- (9CI) (CA INDEX NAME)



L95 ANSWER 16 OF 30 HCAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1994:77181 HCAPLUS
 DOCUMENT NUMBER: 120:77181
 TITLE: Preparation of hexahydroazepine derivatives as 5-HT1A
 serotonergic receptor antagonists
 INVENTOR(S): Takahashi, Nobuyuki; Suzuki, Yukio; Mochizuki,
 Daisuke; Tsujita, Ryuichi; Yaso, Masao; Komaki,
 Hisayuki
 PATENT ASSIGNEE(S): Asahi Kasei Kogyo K. K., Japan
 SOURCE: PCT Int. Appl., 145 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9311116	A1	19930610	WO 1992-JP1533	19921124
W: CA, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
JP 05345764	A2	19931227	JP 1992-307377	19921117
PRIORITY APPLN. INFO.:			JP 1991-336053	A 19911126
			JP 1992-307377	A 19921117
OTHER SOURCE(S):		CASREACT 120:77181; MARPAT 120:77181		
GI				



AB The title compds. [I; R1 = (un)substituted hexahydroazepin-1-yl; R2 = (un)substituted Ph, e.g., (trifluoromethyl)phenyl, (un)substituted pyridazinyl or 1,2-benzisothiazolyl; n = 2-5 integer; m = 2, 3], 5-HT1A

serotonergic receptors and therefore useful for treatment of many ailments, e.g., anxiety, depression, motion sickness, hypertension (no data), are prepared E.g., caprolactam was treated with Cl-(CH₂)₃-Br in THF containing NaH at room temperature for 5 h to give

1-(3-chloropropyl)hexahydro-1H-azepine, which was refluxed with 1-[3-(trifluoromethyl)phenyl]piperazine in benzene containing Et₃N for 139 h to give I [R₁ = hexahydro-1H-azepin-1-yl, R₂ = 3-(trifluoromethyl)phenyl, n = 3, m = 2], which had an affinity (K_i) of 13.7 nM for 5-HT_{1A} receptors.

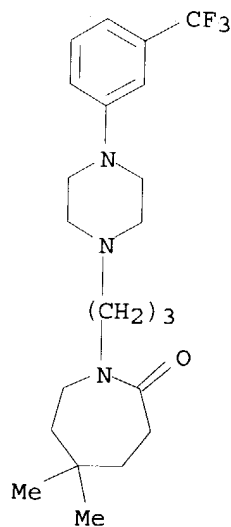
ED Entered STN: 19 Feb 1994

IT 151142-02-8P 151142-03-9P 151142-04-0P
 151142-05-1P 151142-06-2P 151142-07-3P
 151142-08-4P 151142-09-5P 151142-10-8P
 151142-11-9P 151142-17-5P 151142-18-6P
 151142-19-7P 151142-20-0P 151142-21-1P
 151142-22-2P 151142-23-3P 151142-24-4P
 151142-25-5P 151142-26-6P 151142-27-7P
 151142-54-0P 151142-72-2P 151142-73-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, as serotonergic receptor antagonist)

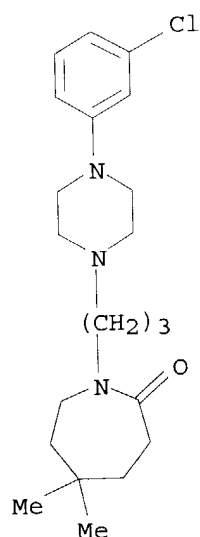
RN 151142-02-8 HCAPLUS

CN 2H-Azepin-2-one, hexahydro-5,5-dimethyl-1-[3-[4-[3-(trifluoromethyl)phenyl]-1-piperazinyl]propyl]- (9CI) (CA INDEX NAME)

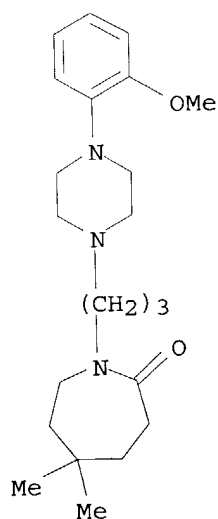


RN 151142-03-9 HCAPLUS

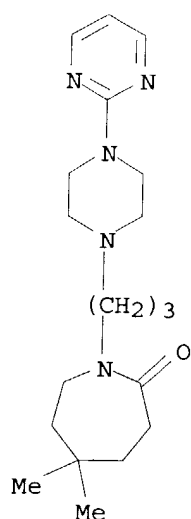
CN 2H-Azepin-2-one, 1-[3-[4-(3-chlorophenyl)-1-piperazinyl]propyl]hexahydro-5,5-dimethyl- (9CI) (CA INDEX NAME)



RN 151142-04-0 HCAPLUS
 CN 2H-Azepin-2-one, hexahydro-1-[3-[4-(2-methoxyphenyl)-1-piperazinyl]propyl]-5,5-dimethyl- (9CI) (CA INDEX NAME)

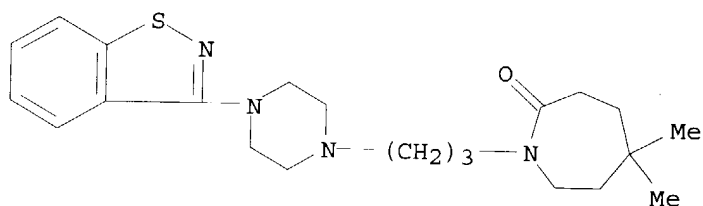


RN 151142-05-1 HCAPLUS
 CN 2H-Azepin-2-one, hexahydro-5,5-dimethyl-1-[3-[4-(2-pyrimidinyl)-1-piperazinyl]propyl]- (9CI) (CA INDEX NAME)



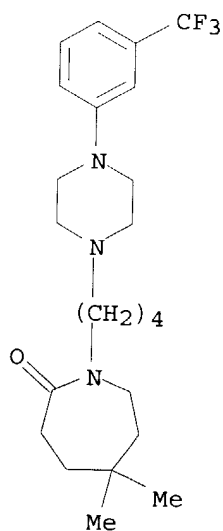
RN 151142-06-2 HCAPLUS

CN 2H-Azepin-2-one, 1-[3-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]propyl]hexahydro-5,5-dimethyl- (9CI) (CA INDEX NAME)

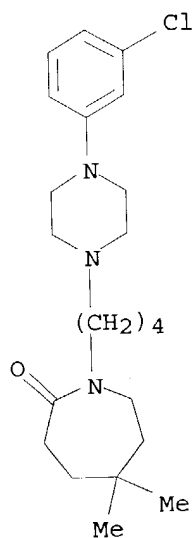


RN 151142-07-3 HCAPLUS

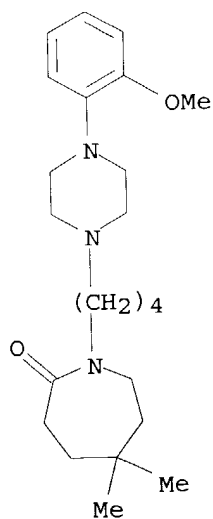
CN 2H-Azepin-2-one, hexahydro-5,5-dimethyl-1-[4-[4-[3-(trifluoromethyl)phenyl]-1-piperazinyl]butyl]- (9CI) (CA INDEX NAME)



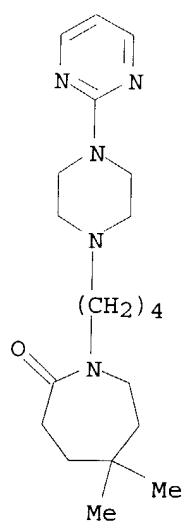
RN 151142-08-4 HCAPLUS
 CN 2H-Azepin-2-one, 1-[4-[4-(3-chlorophenyl)-1-piperazinyl]butyl]hexahydro-
 5,5-dimethyl- (9CI) (CA INDEX NAME)



RN 151142-09-5 HCAPLUS
 CN 2H-Azepin-2-one, hexahydro-1-[4-[4-(2-methoxyphenyl)-1-piperazinyl]butyl]-
 5,5-dimethyl- (9CI) (CA INDEX NAME)

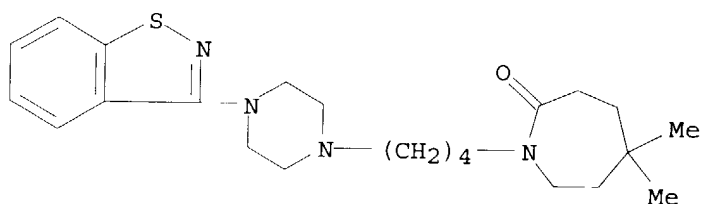


RN 151142-10-8 HCAPLUS
 CN 2H-Azepin-2-one, hexahydro-5,5-dimethyl-1-[4-[4-(2-pyrimidinyl)-1-
 piperazinyl]butyl]- (9CI) (CA INDEX NAME)



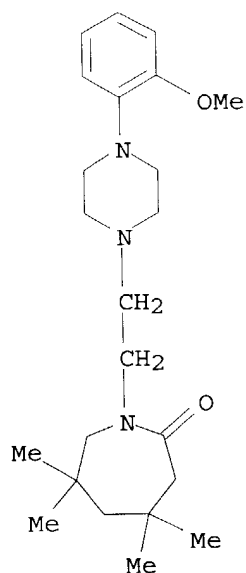
RN 151142-11-9 HCAPLUS

CN 2H-Azepin-2-one, 1-[4-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]butyl]hexahydro-5,5-dimethyl- (9CI) (CA INDEX NAME)

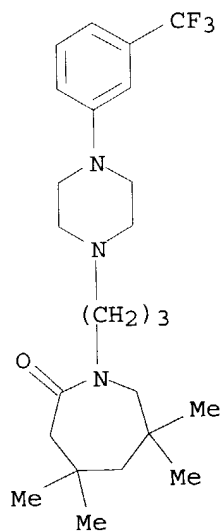


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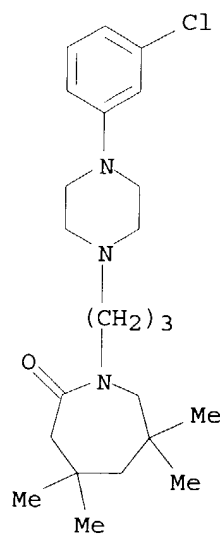
CN 2H-Azepin-2-one, hexahydro-1-[2-[4-(2-methoxyphenyl)-1-piperazinyl]ethyl]-4,4,6,6-tetramethyl- (9CI) (CA INDEX NAME)



RN 151142-18-6 HCAPLUS
 CN 2H-Azepin-2-one, hexahydro-4,4,6,6-tetramethyl-1-[3-[4-[3-(trifluoromethyl)phenyl]-1-piperazinyl]propyl]- (9CI) (CA INDEX NAME)

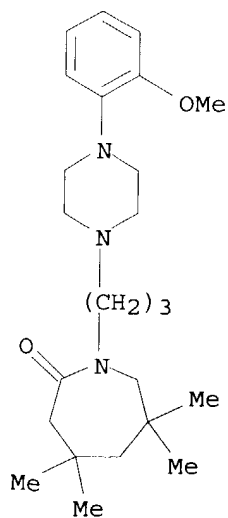


RN 151142-19-7 HCAPLUS
 CN 2H-Azepin-2-one, 1-[3-[4-(3-chlorophenyl)-1-piperazinyl]propyl]hexahydro-4,4,6,6-tetramethyl- (9CI) (CA INDEX NAME)



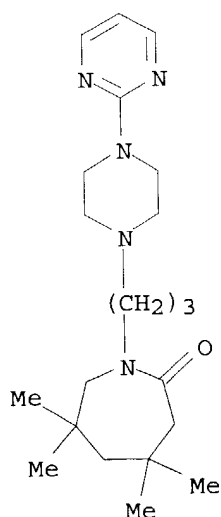
RN 151142-20-0 HCAPLUS

CN 2H-Azepin-2-one, hexahydro-1-[3-[4-(2-methoxyphenyl)-1-piperazinyl]propyl]-4,4,6,6-tetramethyl- (9CI) (CA INDEX NAME)

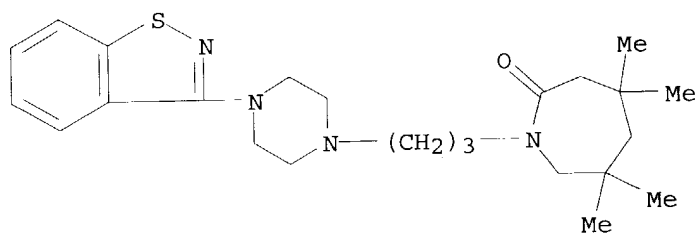


RN 151142-21-1 HCAPLUS

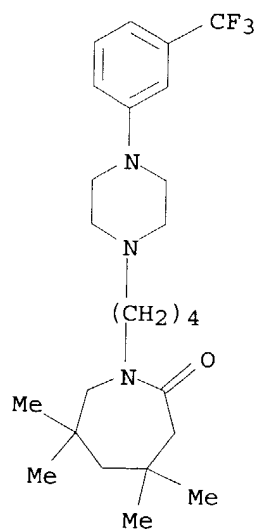
CN 2H-Azepin-2-one, hexahydro-4,4,6,6-tetramethyl-1-[3-[4-(2-pyrimidinyl)-1-piperazinyl]propyl]- (9CI) (CA INDEX NAME)



RN 151142-22-2 HCAPLUS
 CN 2H-Azepin-2-one, 1-[3-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]propyl]hexahydro-4,4,6,6-tetramethyl- (9CI) (CA INDEX NAME)

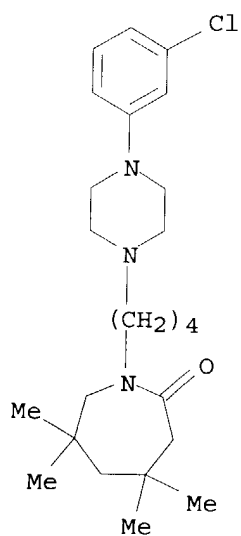


RN 151142-23-3 HCAPLUS
 CN 2H-Azepin-2-one, hexahydro-4,4,6,6-tetramethyl-1-[4-[3-(trifluoromethyl)phenyl]-1-piperazinyl]butyl]- (9CI) (CA INDEX NAME)



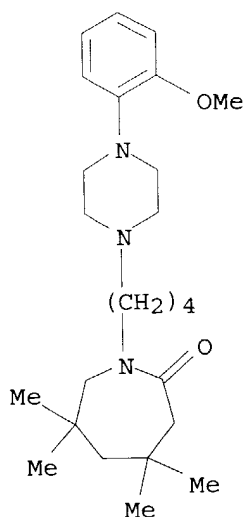
RN 151142-24-4 HCAPLUS

CN 2H-Azepin-2-one, 1-[4-[4-(3-chlorophenyl)-1-piperazinyl]butyl]hexahydro-4,4,6,6-tetramethyl- (9CI) (CA INDEX NAME)

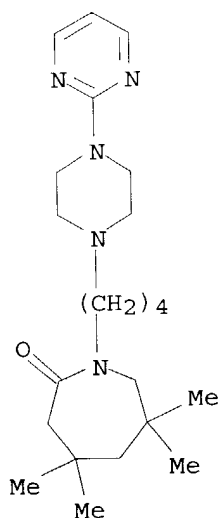


RN 151142-25-5 HCAPLUS

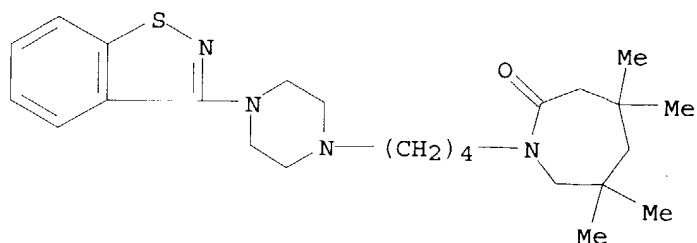
CN 2H-Azepin-2-one, hexahydro-1-[4-[4-(2-methoxyphenyl)-1-piperazinyl]butyl]-4,4,6,6-tetramethyl- (9CI) (CA INDEX NAME)



RN 151142-26-6 HCAPLUS
 CN 2H-Azepin-2-one, hexahydro-4,4,6,6-tetramethyl-1-[4-[4-(2-pyrimidinyl)-1-piperazinyl]butyl]- (9CI) (CA INDEX NAME)

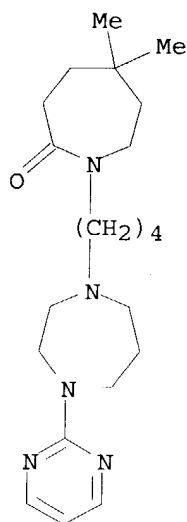


RN 151142-27-7 HCAPLUS
 CN 2H-Azepin-2-one, 1-[4-[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]butyl]hexahydro-4,4,6,6-tetramethyl- (9CI) (CA INDEX NAME)



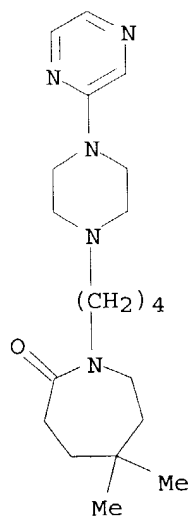
RN 151142-54-0 HCAPLUS

CN 2H-Azepin-2-one, 1-[4-[hexahydro-4-(2-pyrimidinyl)-1H-1,4-diazepin-1-yl]butyl]hexahydro-5,5-dimethyl- (9CI) (CA INDEX NAME)

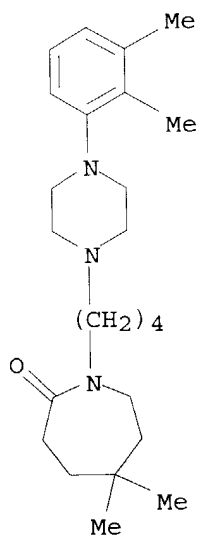


RN 151142-72-2 HCAPLUS

CN 2H-Azepin-2-one, hexahydro-5,5-dimethyl-1-[4-(4-pyrazinyl-1-piperazinyl)butyl]- (9CI) (CA INDEX NAME)



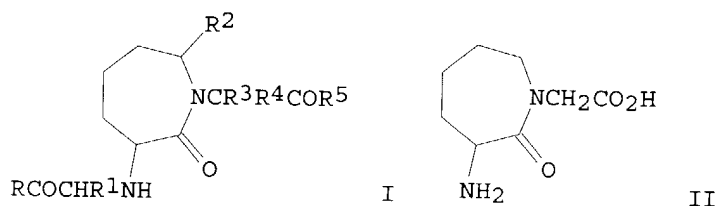
RN 151142-73-3 HCAPLUS
CN 2H-Azepin-2-one, 1-[4-[4-(2,3-dimethylphenyl)-1-piperazinyl]butyl]hexahydro-5,5-dimethyl- (9CI) (CA INDEX NAME)



L95 ANSWER 17 OF 30 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1982:217724 HCAPLUS
DOCUMENT NUMBER: 96:217724
TITLE: Substituted caprolactam derivatives as
antihypertensives, pharmaceutical composition
containing them, and intermediates
INVENTOR(S): Harris, Elbert E.; Patchett, Arthur A.; Thorsett,
Eugene D.
PATENT ASSIGNEE(S): Merck and Co., Inc. , USA
SOURCE: Eur. Pat. Appl., 94 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent

LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 46291	A2	19820224	EP 1981-106372	19810817
EP 46291	A3	19820414		
EP 46291	B1	19851227		
R: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE				
DK 8103641	A	19820219	DK 1981-3641	19810817
ES 504791	A1	19830401	ES 1981-504791	19810817
JP 57112373	A2	19820713	JP 1981-128293	19810818
JP 02054342	B4	19901121		
NO 8103627	A	19830114	NO 1981-3627	19811027
FI 8103378	A	19830114	FI 1981-3378	19811028
ZA 8107685	A	19821027	ZA 1981-7685	19811106
US 4629787	A	19861216	US 1982-394749	19820702
ES 519057	A1	19840316	ES 1983-519057	19830117
US 4680392	A	19870714	US 1986-864234	19860519
PRIORITY APPLN. INFO.:			US 1980-179305	A 19800818
			US 1981-282580	A 19810713
			US 1982-394749	A2 19820702
OTHER SOURCE(S):		CASREACT 96:217724		
GI				



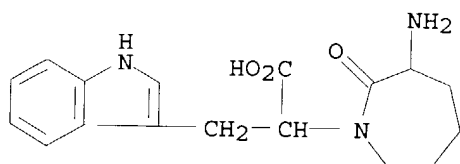
AB Antihypertensive (no data) caprolactams I [R, R5 = OH, (un)substituted alkoxy, aryloxy, amino; R1 = H, (un)substituted alkyl; R2 = H, (un)substituted alkyl, aryl, heteroaryl; R3 = H, (un)substituted alkyl, Ph; R4 = H, alkyl] were prepared. Thus I (R = R5 = OH, R1 = CH2CH2Ph, R2-R4 = H) was prepared by reductive alkylation of the amine II with PhCH2CH2COCO2H. The amine was prepared from protected lysine in 4 steps.

ED Entered STN: 12 May 1984

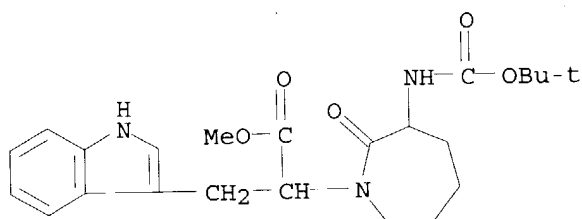
IT **81867-57-4P**
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and alkylation of)

RN 81867-57-4 HCAPLUS

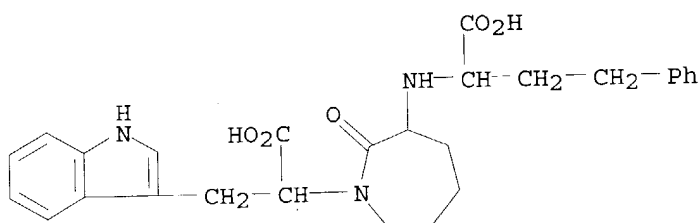
CN 1H-Indole-3-propanoic acid, α -(3-aminoheptahydro-2-oxo-1H-azepin-1-yl)- (9CI) (CA INDEX NAME)



IT **81867-56-3P**
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and saponification of)
 RN 81867-56-3 HCAPLUS
 CN 1H-Indole-3-propanoic acid, α -[3-[[[(1,1-dimethylethoxy)carbonyl]amino]hexahydro-2-oxo-1H-azepin-1-yl]-, methyl
 ester (9CI) (CA INDEX NAME)

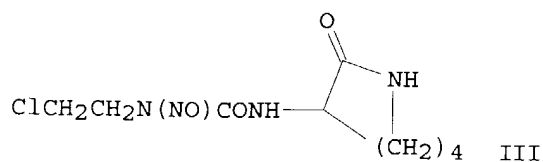
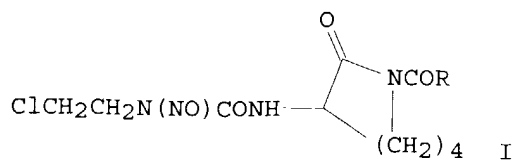


IT **81867-58-5P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 81867-58-5 HCAPLUS
 CN 1H-Indole-3-propanoic acid, α -[3-[(1-carboxy-3-phenylpropyl)amino]hexahydro-2-oxo-1H-azepin-1-yl]- (9CI) (CA INDEX NAME)



L95 ANSWER 18 OF 30 HCAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1978:443156 HCAPLUS
 DOCUMENT NUMBER: 89:43156
 TITLE: Nitrosoarea derivatives
 INVENTOR(S): Matsumoto, Jun; Murakami, Masuo; Sato, Noriaki;
 Hashimoto, Shinichi; Kawamura, Tsutomu; Ichikawa,
 Kaichiro
 PATENT ASSIGNEE(S): Yamanouchi Pharmaceutical Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 53034790	A2	19780331	JP 1976-109628	19760913
PRIORITY APPLN. INFO.: GI			JP 1976-109628	19760913



AB Nitrosoarea derivs. I [R = 2-phenyl-2H-1,2,3-triazol-4-yl (II), 1-phenylpyrazol-5-yl, 4-methylphthalazan-3-yl, 1-adamantyl, 4-chloro-2-phenylpyrimidin-5-yl, Pr2NCO, 2,6-dioxopiperidin-4-ylmethyl, MeO2C] were prepared by silylation of III followed by reaction of RCOX (X = halo). I had antileukemic and anticarcinogenic activities (no data). Thus, 1.68 mL Et3N in dioxane was added to a mixture of 2.62 g III and 1.29 g Me3SiCl in dioxane, the whole stirred 20 h at room temperature, filtered, and the filtrate concentrated to give 10 mL solution;

2-phenyl-1,2,3-triazol-4-carbonyl chloride (1.5 g) in CH₂Cl₂ was added to 6 mL of the solution and the mixture stirred 3 days at room temperature to give 165 mg II.

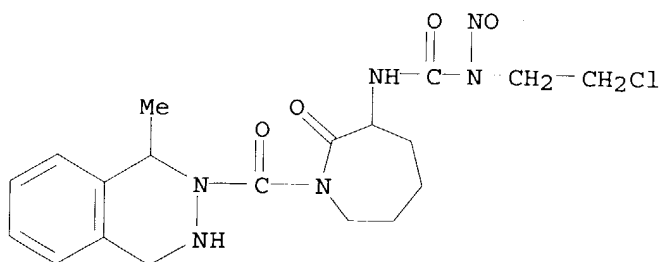
ED Entered STN: 12 May 1984

IT 67060-43-9P 67060-44-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

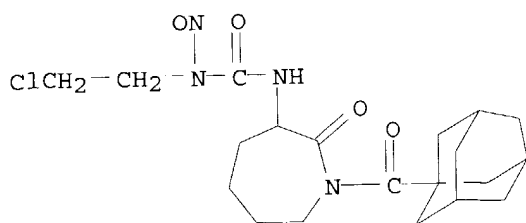
RN 67060-43-9 HCAPLUS

CN Phthalazine, 2-[[[3-[[[(2-chloroethyl)nitrosoamino]carbonyl]amino]hexahydro-2-oxo-1H-azepin-1-yl]carbonyl]-1,2,3,4-tetrahydro-1-methyl- (9CI) (CA INDEX NAME)



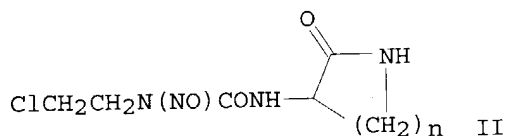
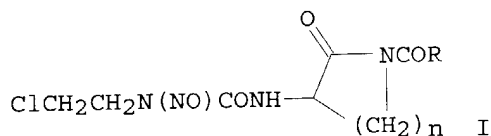
RN 67060-44-0 HCAPLUS

CN 2H-Azepin-2-one, 3-[[[(2-chloroethyl)nitrosoamino]carbonyl]amino]hexahydro-
1-(tricyclo[3.3.1.1^{3,7}]dec-1-ylcarbonyl)- (9CI) (CA INDEX NAME)



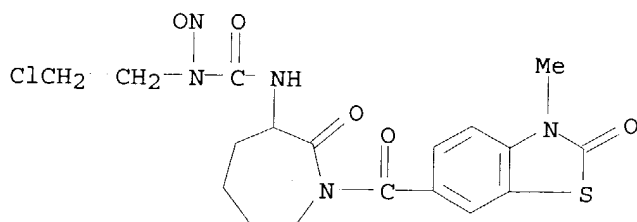
L95 ANSWER 19 OF 30 HCAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1978:6756 HCAPLUS
 DOCUMENT NUMBER: 88:6756
 TITLE: Nitroso urea derivatives
 INVENTOR(S): Murakami, Masuo; Ichikawa, Kaichiro; Matsumoto, Atsushi; Sato, Norio; Hashimoto, Shinichi; Kawamura, Tsutomu
 PATENT ASSIGNEE(S): Yamanouchi Pharmaceutical Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 14 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 52083747	A2	19770712	JP 1976-283	19760101
PRIORITY APPLN. INFO.: GI			JP 1976-283	19760101



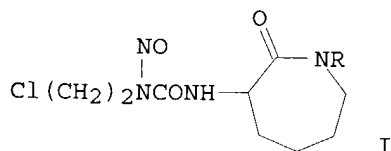
AB Twenty-eight title derivs. I [R = halo, substituted alkyl, (un)substituted alkenyl, (un)substituted aryl, (un)substituted heterocyclics; n = 2-10] were prepared by reaction of II with RCOX (X = halo). I had antitumor activity (some data given in mice). Thus, 174 mg 4-ClC6H4COCl in CHCl3 was added to 440 mg 1-(β-chloroethyl)-3-(2-oxo-3-hexahydroazepinyl)-1-nitroso-urea mercuric salt in CHCl3 at room temperature and the mixture stirred 3 h to give 204 mg 1-(β-chloroethyl)-3-(N-p-chlorobenzoyl-2-oxo-3-hexahydroazepinyl)-1-nitroso-urea.
 ED Entered STN: 12 May 1984
 IT 63847-31-4P
 RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)
 RN 63847-31-4 HCAPLUS
 CN 2H-Azepin-2-one, 3-[[[(2-chloroethyl)nitrosoamino]carbonyl]amino]-1-[(2,3-dihydro-3-methyl-2-oxo-6-benzothiazolyl)carbonyl]hexahydro- (9CI) (CA INDEX NAME)



L95 ANSWER 20 OF 30 HCAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1977:535119 HCAPLUS
 DOCUMENT NUMBER: 87:135119
 TITLE: 1-(β-Chloroethyl)-3-substituted 1-nitrosoureas
 INVENTOR(S): Murakami, Masuo; Ichikawa, Kaichiro; Matsumoto, Jun; Sato, Norio; Hashimoto, Shinichi; Kawamura, Tsutomu
 PATENT ASSIGNEE(S): Yamanouchi Pharmaceutical Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 52051363	A2	19770425	JP 1975-127807	19751023
PRIORITY APPLN. INFO.: GI			JP 1975-127807	19751023



AB Thirteen title compds. (I, R = acyl) remedies for tumors, were prepared by treating non-substituted I with a silylating agent followed by acylation. Thus, 2.62 g 1-(β-chloroethyl)-3-(2-oxo-3-hexahydroazepinyl)-1-nitrosourea and Me₃SiCl in dioxane were treated with NEt₃ and treated with 352 mg p-[bis(β-chloroethyl)amino]benzoyl chloride in dichloromethane to give 403 mg I [R = p-[bis(β-chloroethyl)amino]benzoyl]. Among 12 I similarly prepared were (R given): 4-oxo-4H-thiopyran-3-carbonyl, p-O₂NC₆H₄CO, p-(dimethylamino)benzoyl, 3-methyl-2-oxo-2,3-dihydrobenzothiazole-6-carbonyl.

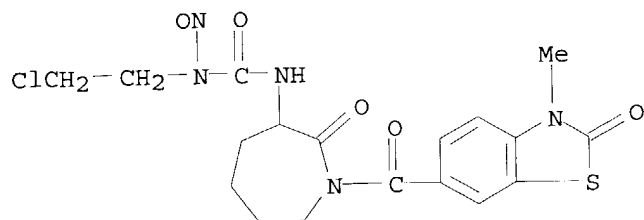
ED Entered STN: 12 May 1984

IT 63847-31-4P 64148-23-8P

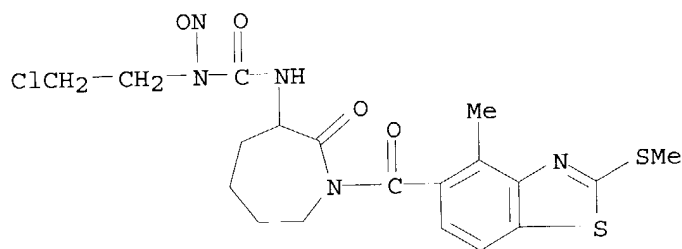
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 63847-31-4 HCAPLUS
 CN 2H-Azepin-2-one, 3-[[[(2-chloroethyl)nitrosoamino]carbonyl]amino]-1-[(2,3-dihydro-3-methyl-2-oxo-6-benzothiazolyl)carbonyl]hexahydro- (9CI) (CA INDEX NAME)

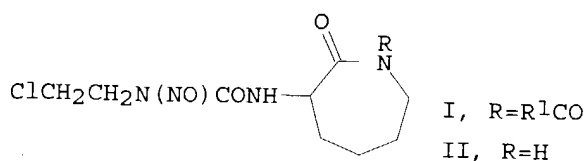


RN 64148-23-8 HCAPLUS
 CN 2H-Azepin-2-one, 3-[[[(2-chloroethyl)nitrosoamino]carbonyl]amino]hexahydro-1-[[4-methyl-2-(methylthio)-5-benzothiazolyl]carbonyl]- (9CI) (CA INDEX NAME)



L95 ANSWER 21 OF 30 HCAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1977:502197 HCAPLUS
 DOCUMENT NUMBER: 87:102197
 TITLE: Nitrosoarea derivatives
 INVENTOR(S): Murakami, Masuo; Ichikawa, Kaichiro; Matsumoto, Jun;
 Sato, Norio; Hashimoto, Shinichi; Kawamura, Tsutomu
 PATENT ASSIGNEE(S): Yamanouchi Pharmaceutical Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 52046072	A2	19770412	JP 1975-121967	19751008
PRIORITY APPLN. INFO.: GI			JP 1975-121967	19751008



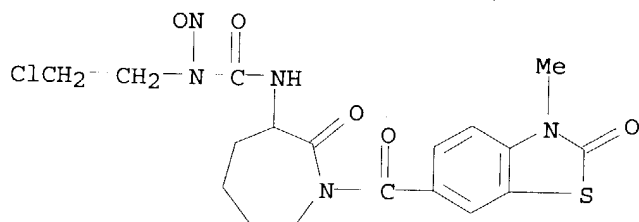
AB Fifteen nitrosourea derivs. I [R¹ = (un)substituted Ph, furyl, pyrazinyl, H₂C:CH, PhCH₂, ClCH₂, etc.] were prepared by reaction of II with R¹COX (X = halo). I had anticancer activity (some data given in mice). Thus, 124 mg 4-ClC₆H₄COCl in CHCl₃ was added to 440 mg II HgCl₂ salt in CHCl₃ and the mixture stirred 3 h at room temperature to give 204 mg I (R¹ = 4-ClC₆H₄).

ED Entered STN: 12 May 1984

IT **63847-31-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and anticarcinogenic activity of)

RN 63847-31-4 HCAPLUS

CN 2H-Azepin-2-one, 3-[[[(2-chloroethyl)nitrosoamino]carbonyl]amino]-1-[(2,3-dihydro-3-methyl-2-oxo-6-benzothiazolyl)carbonyl]hexahydro- (9CI) (CA INDEX NAME)



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YOU HAVE REQUESTED DATA FROM 9 ANSWERS - CONTINUE? Y/(N):y

L95 ANSWER 22 OF 30 USPATFULL on STN

ACCESSION NUMBER: 2004:83481 USPATFULL

TITLE: Microbiocidal n-phenyl-n-[4-(4-pyridyl-2-pyrimidin-2-yl)]-amine derivatives

INVENTOR(S): Eberle, Martin, Basel, SWITZERLAND
Ziegler, Hugo, Basel, SWITZERLAND
Cederbaum, Fredrik, Basel, SWITZERLAND
Ackermann, Peter, Basel, SWITZERLAND
Schnyder, Anita, Basel, SWITZERLAND

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 2004063937	A1	20040401
APPLICATION INFO.:	US 2003-451930	A1	20030625 (10)
	WO 2001-IB2821		20011220

	NUMBER	DATE
PRIORITY INFORMATION:	GB 2001-102	20010103
DOCUMENT TYPE:	Utility	

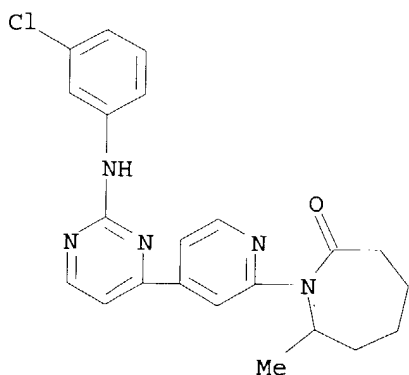
FILE SEGMENT: APPLICATION
LEGAL REPRESENTATIVE: SYNGENTA CROP PROTECTION, INC., PATENT AND TRADEMARK
DEPARTMENT, 410 SWING ROAD, GREENSBORO, NC, 27409
NUMBER OF CLAIMS: 15
EXEMPLARY CLAIM: 1
LINE COUNT: 1761

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The invention relates to novel N-phenyl-4-(4-pyridyl)-2-pyrimidineamine derivatives of the general formula (1) wherein the sum of (m+p) together is 0, 1, 2 or 3; n and q are independently of each other 0 or 1, and the sum of (m+p+q) together is 1, 2, 3 or 4; R.sub.1 is hydrogen, halogen, alkoxy, haloalkyl, haloalkoxy or alkyl; R.sub.2 is hydrogen, C.sub.1-C.sub.6-alkyl, C.sub.1-C.sub.6-haloalkyl or C.sub.1-C.sub.6-alkoxy; R.sub.2A is hydrogen, C.sub.1-C.sub.6-alkyl, C.sub.3-C.sub.4-alkenyl or C.sub.3-C.sub.4-alkynyl; each of R.sub.3, R.sub.4, R.sub.5 and R.sub.6 is, independently of the others, hydrogen, C.sub.1-C.sub.6-alkyl, C.sub.1-C.sub.6-haloalkyl, hydroxy-C.sub.1-C.sub.6-alkyl or C.sub.1-C.sub.6-alkoxy-C.sub.1-C.sub.6-alkyl, or the ring members CR.sub.3R.sub.4 or CR.sub.5R.sub.6 or CR.sub.2R.sub.2A are independently of each other a carbonyl group (C.dbd.O) or a group C.dbd.S; X is C.dbd.O, C.dbd.S, S.dbd.O or O.dbd.S=O; Y is O, S, C.dbd.O, CH.sub.2A, --N(R.sub.8)--, --O--N(R.sub.8)--, --N(R.sub.8)--O-- or NH--; R.sub.7 is hydrogen, C.sub.1-C.sub.4-alkyl, C.sub.3-C.sub.4-alkenyl, C.sub.3-C.sub.4-alkynyl, --CH.sub.2OR.sub.8, CH.sub.2SR.sub.8, --C(O)R.sub.8, --C(O)OR.sub.8, SO2R.sub.8, SOR.sub.8 or SR.sub.8; and R.sub.8 is C.sub.1-C.sub.8-alkyl, C.sub.1-C.sub.8-alkoxyalkyl, C.sub.1-C.sub.8 haloalkyl or phenylC.sub.1-C.sub.2-alkyl wherein the phenyl may be substituted by up to three groups selected from halo or C.sub.1-C.sub.4-alkyl; or a salt thereof. The invention also relates to the preparation of the compounds and to agrochemical compositions comprising at least one of those compounds as active ingredient as well as the preparation of the said compositions and to the use of the compounds or of the compositions in controlling or preventing the infestation of plants by phytopathogenic microorganisms, especially fungi.

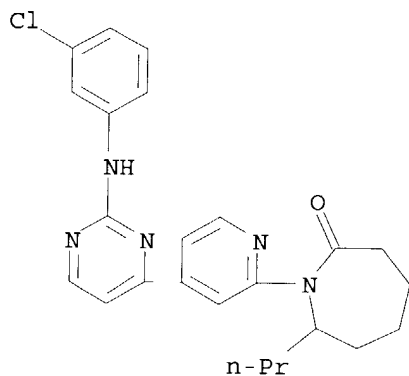
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 442164-61-6P 442164-64-9P 442164-65-0P
442167-54-6P 442167-57-9P 442167-58-0P
442170-53-8P 442170-56-1P 442170-57-2P
442173-70-8P 442173-73-1P 442173-74-2P
442176-64-9P 442176-67-2P 442176-68-3P
442179-79-5P 442179-82-0P 442179-83-1P
442182-73-2P 442182-76-5P 442182-77-6P
442185-71-9P 442185-74-2P 442185-75-3P
442188-69-4P 442188-72-9P 442188-73-0P
442191-84-6P 442191-89-1P 442191-91-5P
(preparation of microbiocidal N-phenyl-N-[4-(4-pyridyl)-pyrimidin-2-yl]amines)
RN 442164-61-6 USPATFULL
CN 2H-Azepin-2-one, 1-[4-[2-[(3-chlorophenyl)amino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-7-methyl- (9CI) (CA INDEX NAME)



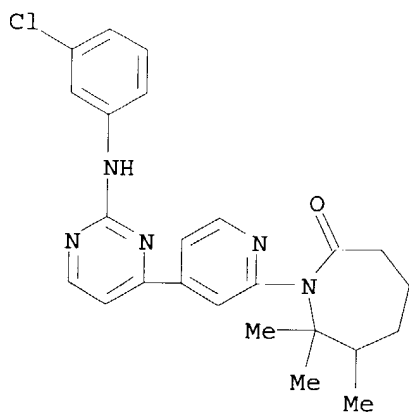
RN 442164-64-9 USPATFULL

CN 2H-Azepin-2-one, 1-[4-[2-[(3-chlorophenyl)amino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-7-propyl- (9CI) (CA INDEX NAME)



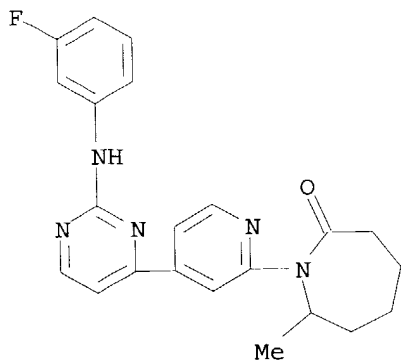
RN 442164-65-0 USPATFULL

CN 2H-Azepin-2-one, 1-[4-[2-[(3-chlorophenyl)amino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-6,7,7-trimethyl- (9CI) (CA INDEX NAME)

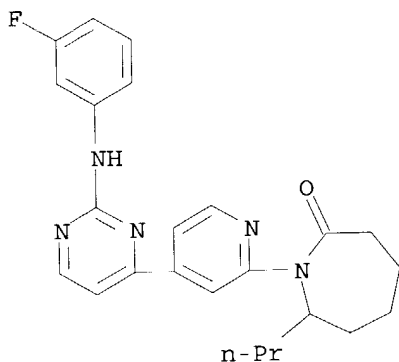


RN 442167-54-6 USPATFULL

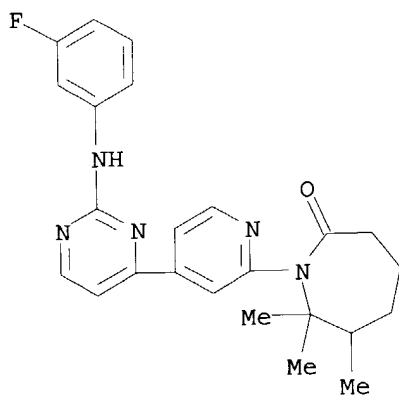
CN 2H-Azepin-2-one, 1-[4-[2-[(3-fluorophenyl)amino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-7-methyl- (9CI) (CA INDEX NAME)



RN 442167-57-9 USPATFULL
 CN 2H-Azepin-2-one, 1-[4-[2-[(3-fluorophenyl)amino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-7-propyl- (9CI) (CA INDEX NAME)

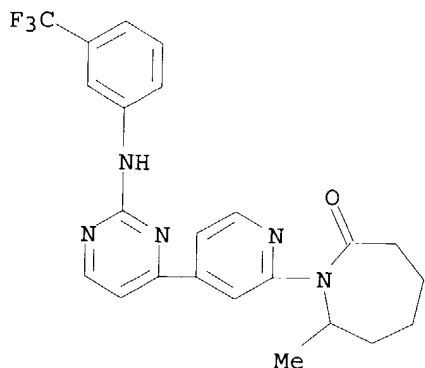


RN 442167-58-0 USPATFULL
 CN 2H-Azepin-2-one, 1-[4-[2-[(3-fluorophenyl)amino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-6,7,7-trimethyl- (9CI) (CA INDEX NAME)



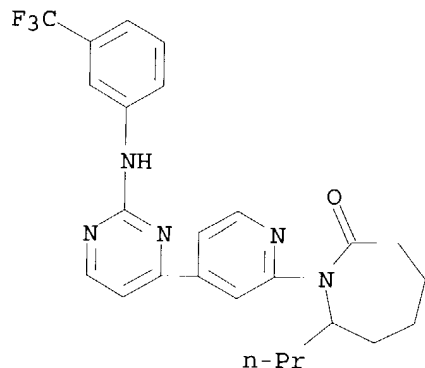
RN 442170-53-8 USPATFULL
 CN 2H-Azepin-2-one, hexahydro-7-methyl-1-[4-[2-[[3-

(trifluoromethyl)phenyl]amino]-4-pyrimidinyl]-2-pyridinyl]- (9CI) (CA
INDEX NAME)



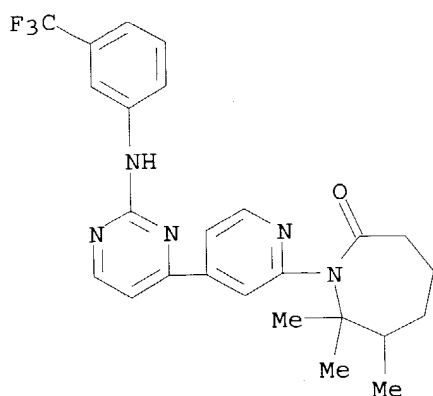
RN 442170-56-1 USPATFULL

CN 2H-Azepin-2-one, hexahydro-7-propyl-1-[4-[2-[[3-(trifluoromethyl)phenyl]amino]-4-pyrimidinyl]-2-pyridinyl]- (9CI) (CA
INDEX NAME)



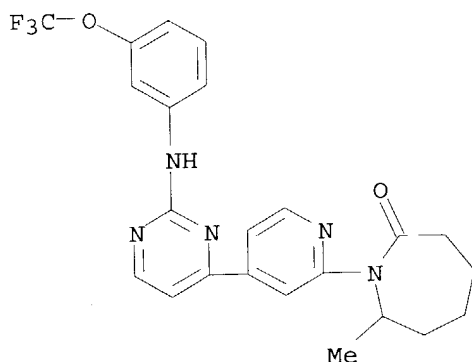
RN 442170-57-2 USPATFULL

CN 2H-Azepin-2-one, hexahydro-6,7,7-trimethyl-1-[4-[2-[[3-(trifluoromethyl)phenyl]amino]-4-pyrimidinyl]-2-pyridinyl]- (9CI) (CA
INDEX NAME)



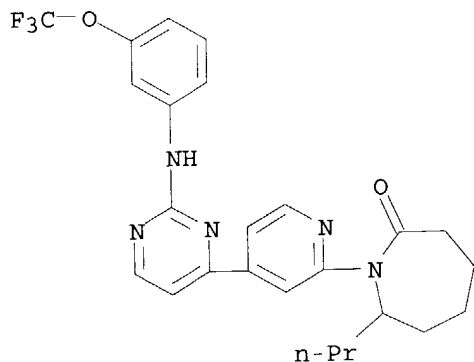
RN 442173-70-8 USPATFULL

CN 2H-Azepin-2-one, hexahydro-7-methyl-1-[4-[2-[[3-(trifluoromethoxy)phenyl]amino]-4-pyrimidinyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



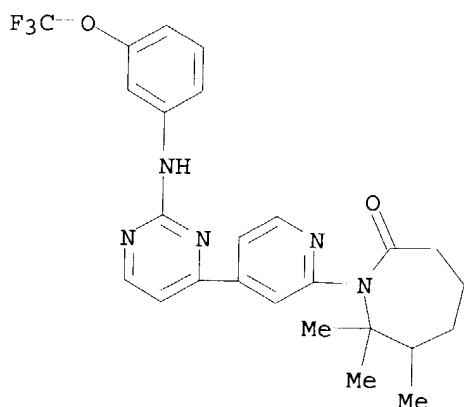
RN 442173-73-1 USPATFULL

CN 2H-Azepin-2-one, hexahydro-7-propyl-1-[4-[2-[[3-(trifluoromethoxy)phenyl]amino]-4-pyrimidinyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



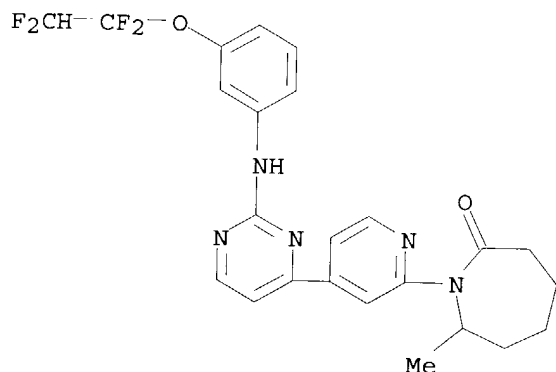
RN 442173-74-2 USPATFULL

CN 2H-Azepin-2-one, hexahydro-6,7,7-trimethyl-1-[4-[2-[[3-(trifluoromethoxy)phenyl]amino]-4-pyrimidinyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



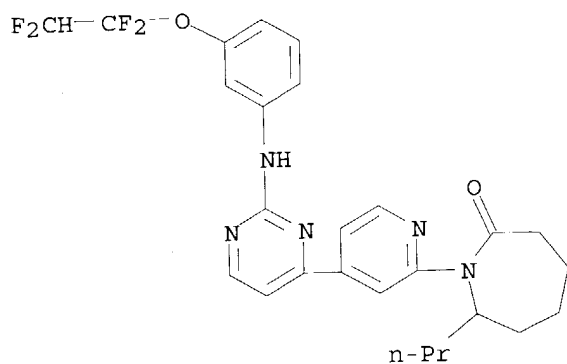
RN 442176-64-9 USPATFULL

CN 2H-Azepin-2-one, hexahydro-7-methyl-1-[4-[2-[[3-(1,1,2,2-tetrafluoroethoxy)phenyl]amino]-4-pyrimidinyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)

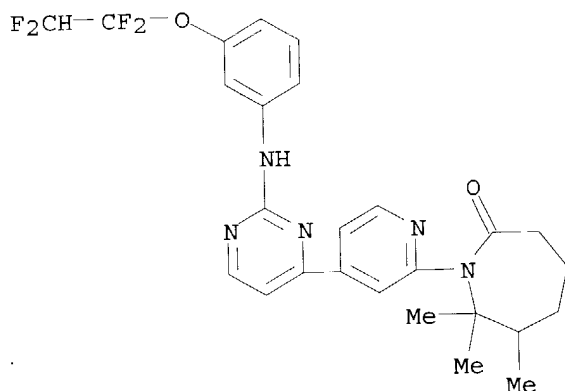


RN 442176-67-2 USPATFULL

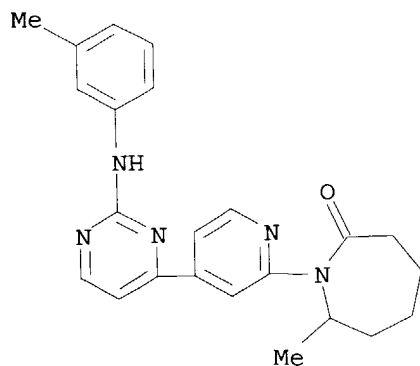
CN 2H-Azepin-2-one, hexahydro-7-propyl-1-[4-[2-[[3-(1,1,2,2-tetrafluoroethoxy)phenyl]amino]-4-pyrimidinyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



RN 442176-68-3 USPATFULL
 CN 2H-Azepin-2-one, hexahydro-6,7,7-trimethyl-1-[4-[2-[[3-(1,1,2,2-tetrafluoroethoxy)phenyl]amino]-4-pyrimidinyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)

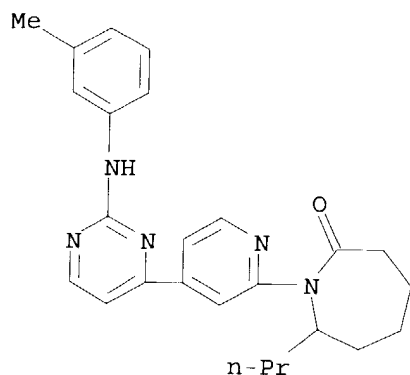


RN 442179-79-5 USPATFULL
 CN 2H-Azepin-2-one, hexahydro-7-methyl-1-[4-[2-[(3-methylphenyl)amino]-4-pyrimidinyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



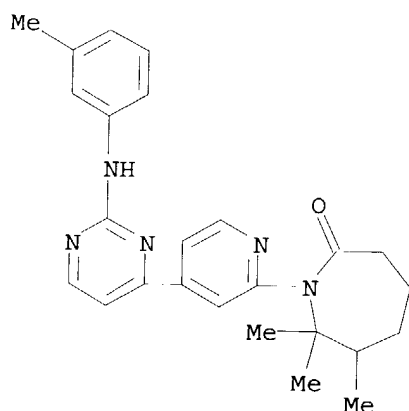
RN 442179-82-0 USPATFULL
 CN 2H-Azepin-2-one, hexahydro-1-[4-[2-[(3-methylphenyl)amino]-4-pyrimidinyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)

2-pyridinyl]-7-propyl- (9CI) (CA INDEX NAME)



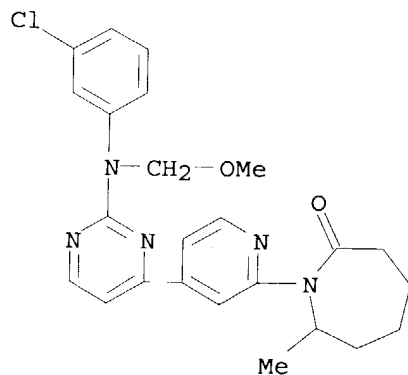
RN 442179-83-1 USPATFULL

CN 2H-Azepin-2-one, hexahydro-6,7,7-trimethyl-1-[4-[2-[(3-methylphenyl)amino]-4-pyrimidinyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



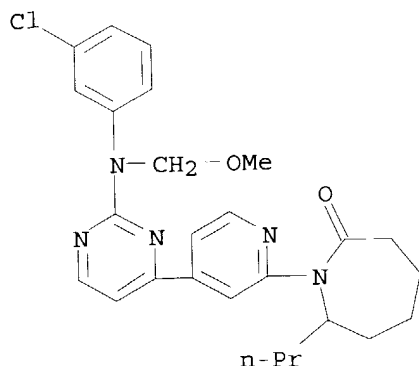
RN 442182-73-2 USPATFULL

CN 2H-Azepin-2-one, 1-[4-[2-[(3-chlorophenyl)(methoxymethyl)amino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-7-methyl- (9CI) (CA INDEX NAME)



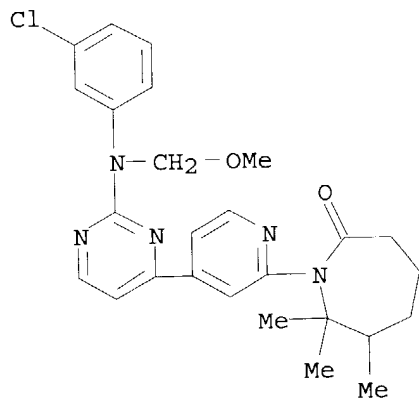
RN 442182-76-5 USPATFULL

CN 2H-Azepin-2-one, 1-[4-[2-[(3-chlorophenyl) (methoxymethyl) amino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-7-propyl- (9CI) (CA INDEX NAME)



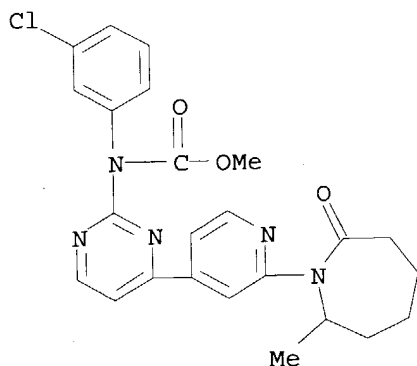
RN 442182-77-6 USPATFULL

CN 2H-Azepin-2-one, 1-[4-[2-[(3-chlorophenyl) (methoxymethyl) amino]-4-pyrimidinyl]-2-pyridinyl]hexahydro-6,7,7-trimethyl- (9CI) (CA INDEX NAME)



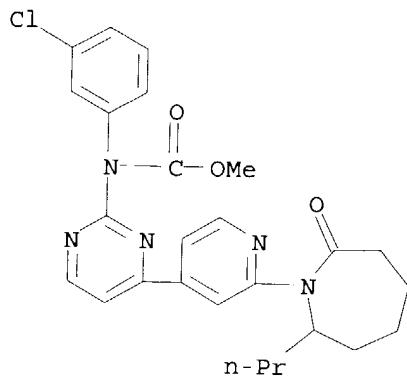
RN 442185-71-9 USPATFULL

CN Carbamic acid, (3-chlorophenyl) [4-[2-(hexahydro-2-methyl-7-oxo-1H-azepin-1-yl)-4-pyridinyl]-2-pyrimidinyl]-, methyl ester (9CI) (CA INDEX NAME)



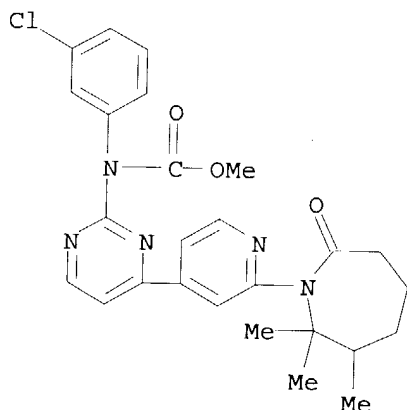
RN 442185-74-2 USPATFULL

CN Carbamic acid, (3-chlorophenyl) [4-[2-(hexahydro-2-oxo-7-propyl-1H-azepin-1-yl)-4-pyridinyl]-2-pyrimidinyl]-, methyl ester (9CI) (CA INDEX NAME)



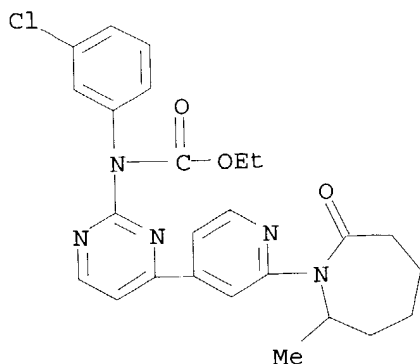
RN 442185-75-3 USPATFULL

CN Carbamic acid, (3-chlorophenyl) [4-[2-(hexahydro-2,2,3-trimethyl-7-oxo-1H-azepin-1-yl)-4-pyridinyl]-2-pyrimidinyl]-, methyl ester (9CI) (CA INDEX NAME)

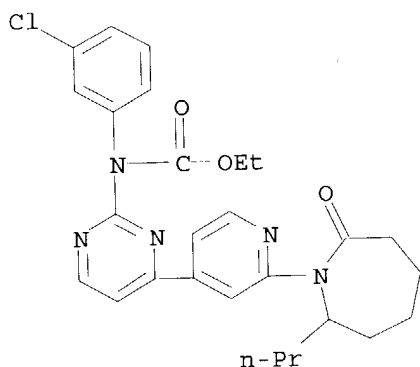


RN 442188-69-4 USPATFULL

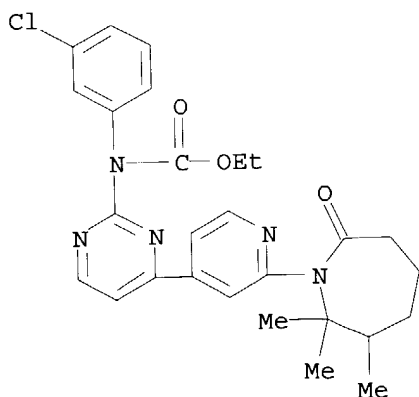
CN Carbamic acid, (3-chlorophenyl) [4-[2-(hexahydro-2-methyl-7-oxo-1H-azepin-1-yl)-4-pyridinyl]-2-pyrimidinyl]-, ethyl ester (9CI) (CA INDEX NAME)



RN 442188-72-9 USPATFULL
 CN Carbamic acid, (3-chlorophenyl) [4-[2-(hexahydro-2-oxo-7-propyl-1H-azepin-1-yl)-4-pyridinyl]-2-pyrimidinyl]-, ethyl ester (9CI) (CA INDEX NAME)

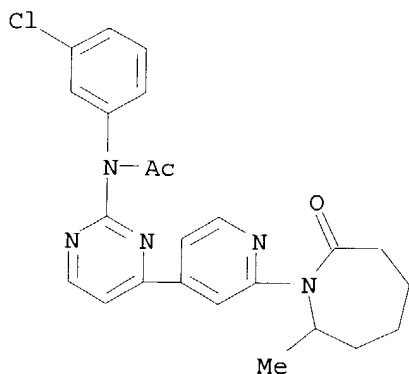


RN 442188-73-0 USPATFULL
 CN Carbamic acid, (3-chlorophenyl) [4-[2-(hexahydro-2,2,3-trimethyl-7-oxo-1H-azepin-1-yl)-4-pyridinyl]-2-pyrimidinyl]-, ethyl ester (9CI) (CA INDEX NAME)



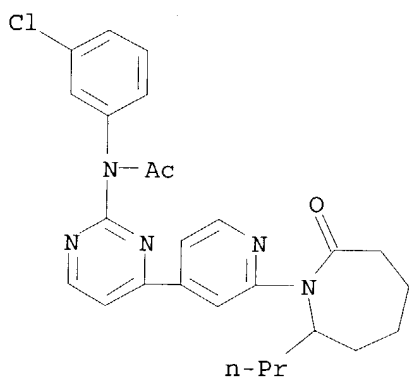
RN 442191-84-6 USPATFULL
 CN Acetamide, N-(3-chlorophenyl)-N-[4-[2-(hexahydro-2-methyl-7-oxo-1H-azepin-

1-yl)-4-pyridinyl]-2-pyrimidinyl]- (9CI) (CA INDEX NAME)



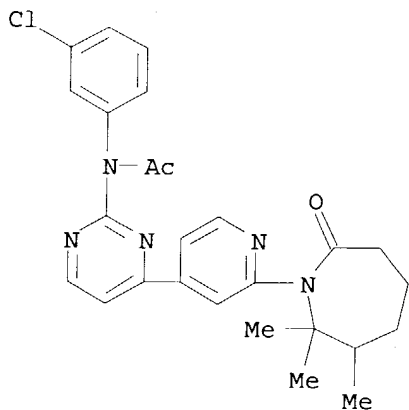
RN 442191-89-1 USPATFULL

CN Acetamide, N-(3-chlorophenyl)-N-[4-[2-(hexahydro-2-oxo-7-propyl-1H-azepin-1-yl)-4-pyridinyl]-2-pyrimidinyl]- (9CI) (CA INDEX NAME)



RN 442191-91-5 USPATFULL

CN Acetamide, N-(3-chlorophenyl)-N-[4-[2-(hexahydro-2,2,3-trimethyl-7-oxo-1H-azepin-1-yl)-4-pyridinyl]-2-pyrimidinyl]- (9CI) (CA INDEX NAME)



L95 ANSWER 23 OF 30 USPATFULL on STN
ACCESSION NUMBER: 2001:168117 USPATFULL
TITLE: Lactam inhibitors of FXa and method
INVENTOR(S): Stein, Philip D., Pennington, NJ, United States
Bisacchi, Gregory S., Ringoes, NJ, United States
Shi, Yan, Flourtown, PA, United States
O'Connor, Stephen P., Lambertville, NJ, United States
Li, Chi, Randolph, NJ, United States
PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, Princeton, NJ, United States (U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 6297233	B1	20011002
APPLICATION INFO.:	US 2000-496571		20000202 (9)
DOCUMENT TYPE:	Utility		
FILE SEGMENT:	GRANTED		
PRIMARY EXAMINER:	Kifle, Bruck		
LEGAL REPRESENTATIVE:	Rodney, Burton		
NUMBER OF CLAIMS:	18		
EXEMPLARY CLAIM:	1		
LINE COUNT:	4323		

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB Caprolactam inhibitors are provided which have the structure ##STR1##

including pharmaceutically acceptable salts thereof and all stereoisomers thereof, and prodrugs thereof, wherein n is 1 to 5; and

and Y R.sup.1, R.sup.2, R.sup.3, R.sup.5, R.sup.5a, R.sup.6, R.sup.7, R.sup.8, R.sup.9 and R.sup.10 are as defined herein. These compounds are inhibitors of Factor Xa and thus are useful as anticoagulants. A method for treating cardiovascular diseases associated with thromboses is also provided.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

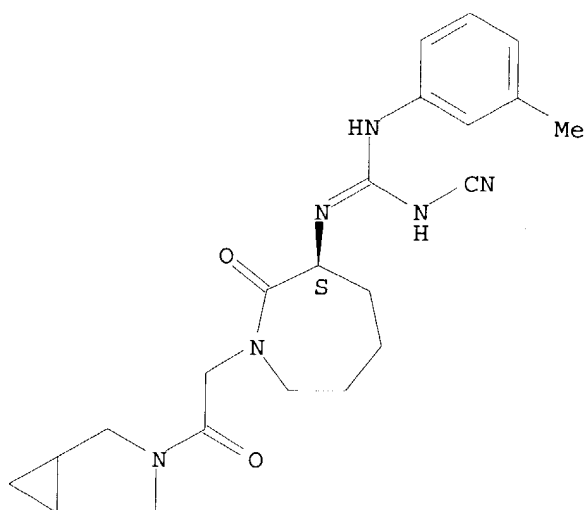
IT 288077-09-8P 288077-32-7P 288077-40-7P
288081-29-8P 288081-35-6P 288081-83-4P
288082-97-3P

(preparation of caprolactams as Factor Xa inhibitors in prevention or treatment of thromboses, coronary artery disease, or cerebrovascular disease in mammals)

RN 288077-09-8 USPATFULL

CN 3-Azabicyclo[3.1.0]hexane, 3-[[[(3S)-3-[[[(cyanoamino)[(3-methylphenyl)amino]methylene]amino]hexahydro-2-oxo-1H-azepin-1-yl]acetyl]- (9CI) (CA INDEX NAME)

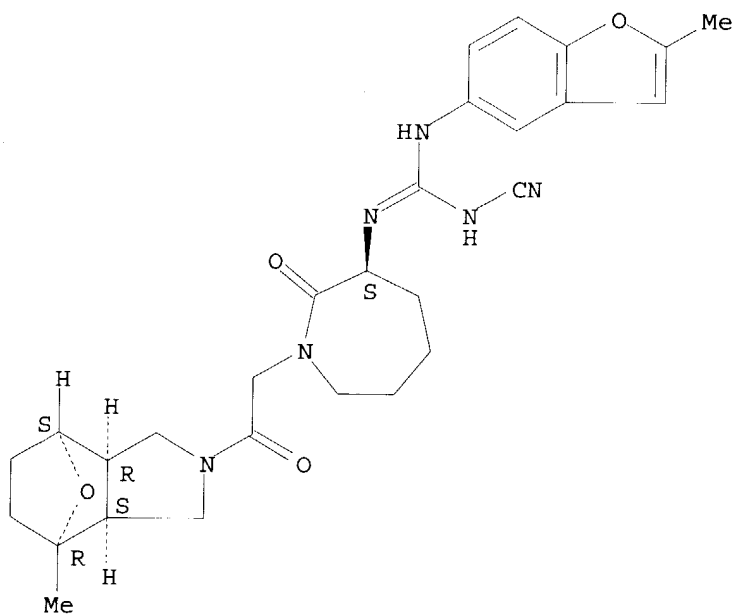
Absolute stereochemistry.



RN 288077-32-7 USPATFULL

CN 4,7-Epoxy-1H-isoindole, 2-[[[(3S)-3-[[[(cyanoamino)[(2-methyl-5-benzofuranyl)amino]methylene]amino]hexahydro-2-oxo-1H-azepin-3-yl]acetyl]octahydro-4-methyl-, (3aS,4R,7S,7aR)- (9CI) (CA INDEX NAME)

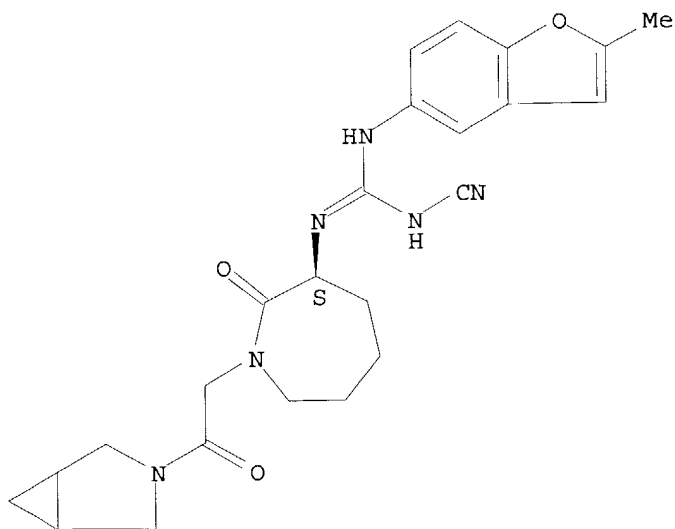
Absolute stereochemistry.



RN 288077-40-7 USPATFULL

CN 3-Azabicyclo[3.1.0]hexane, 3-[[[(3S)-3-[[[(cyanoamino)[(2-methyl-5-benzofuranyl)amino]methylene]amino]hexahydro-2-oxo-1H-azepin-1-yl]acetyl]- (9CI) (CA INDEX NAME)

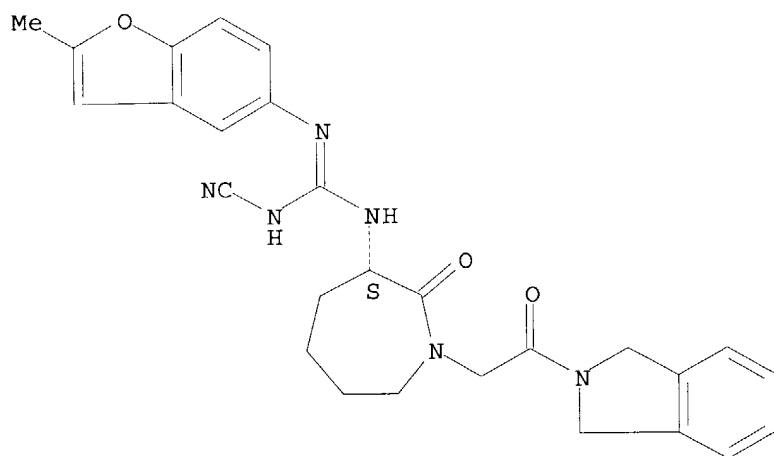
Absolute stereochemistry.



RN 288081-29-8 USPATFULL

CN 1H-Isoindole, 2-[[[(3S)-3-[[[(cyanoamino)[(2-methyl-5-benzofuranyl)amino]methylene]amino]hexahydro-2-oxo-1H-azepin-1-yl]acetyl]-2,3-dihydro- (9CI) (CA INDEX NAME)

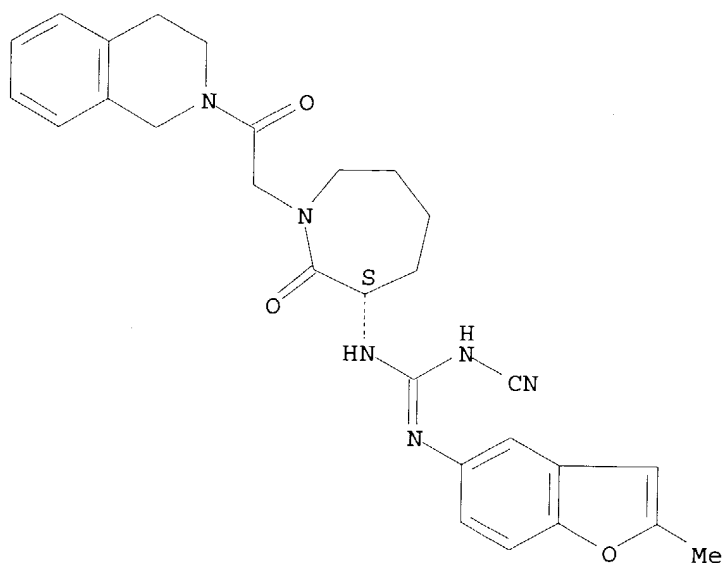
Absolute stereochemistry.



RN 288081-35-6 USPATFULL

CN Isoquinoline, 2-[[[(3S)-3-[[[(cyanoamino)[(2-methyl-5-benzofuranyl)amino]methylene]amino]hexahydro-2-oxo-1H-azepin-1-yl]acetyl]-1,2,3,4-tetrahydro- (9CI) (CA INDEX NAME)

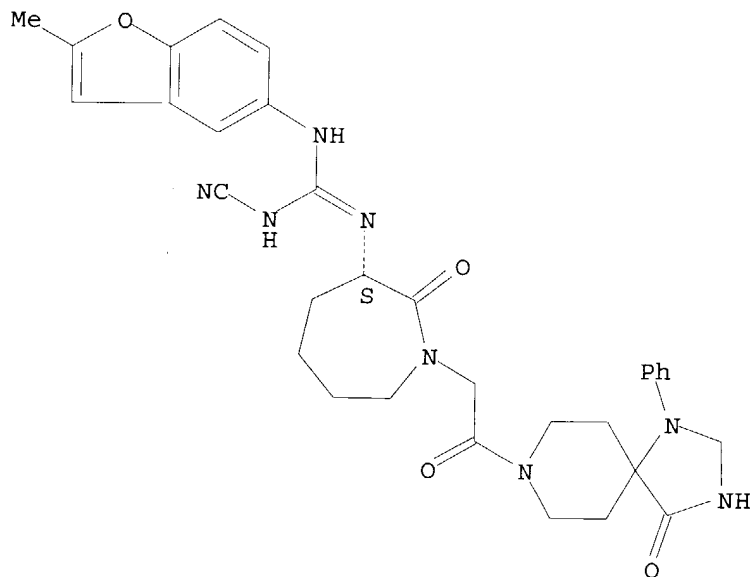
Absolute stereochemistry.



RN 288081-83-4 USPATFULL

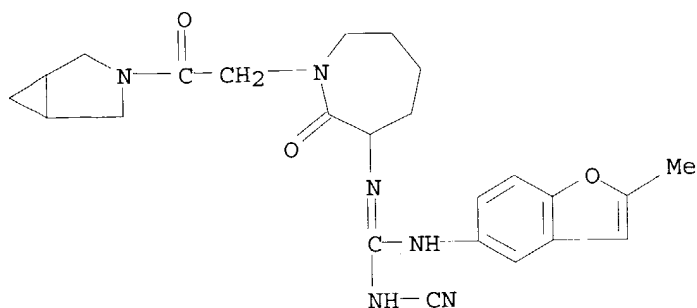
CN 1,3,8-Triazaspiro[4.5]decan-4-one, 8-[[[(3S)-3-[[[(cyanoamino)[(2-methyl-5-benzofuranyl)amino]methylene]amino]hexahydro-2-oxo-1H-azepin-1-yl]acetyl]-1-phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 288082-97-3 USPATFULL

CN 3-Azabicyclo[3.1.0]hexane, 3-[[3-[[[(cyanoamino)[(2-methyl-5-benzofuranyl)amino]methylene]amino]hexahydro-2-oxo-1H-azepin-1-yl]acetyl]- (9CI) (CA INDEX NAME)



L95 ANSWER 24 OF 30 USPATFULL on STN
 ACCESSION NUMBER: 93:18665 USPATFULL
 TITLE: Derivatives of 1,2,3,4-tetrahydronaphthylamine endowed with nootropic activity and pharmaceutical compositions containing same
 INVENTOR(S): Giannessi, Fabio, Rome, Italy
 Ghirardi, Orlando, Rome, Italy
 Misiti, Domenico, Rome, Italy
 Tinti, Maria O., Rome, Italy
 Cozzolino, Roberto, Rome, Italy
 PATENT ASSIGNEE(S): Sigma-Tau Industrie Farmaceutiche Riunite S.p.A., Rome, Italy (non-U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 5192759		19930309
APPLICATION INFO.:	US 1991-809874		19911218 (7)

	NUMBER	DATE
PRIORITY INFORMATION:	IT 1990-48605	19901221
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	Granted	
PRIMARY EXAMINER:	Bond, Robert T.	
LEGAL REPRESENTATIVE:	Allegretti & Witcoff, Ltd.	
NUMBER OF CLAIMS:	4	
EXEMPLARY CLAIM:	1,3	
LINE COUNT:	537	

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB 1,2,3,4-tetrahydronaphthylamines of formula (1) ##STR1## wherein R is H or OCH.sub.3 ; ##STR2## is either at 1 or 2 position R.sub.1 is H;

R.sub.2 is selected from:

L-prolyl, optionally N-substituted with acetyl or carbobenzoxy,

L-pyroglutamyl,

(pyrrolidin-2-one-1-yl)acetyl,

3-carboxy-2-hydroxypropyl:

or R.sub.1 and R.sub.2 taken together with the nitrogen atom form the ring ##STR3## wherein n=1,2,3 and R.sub.3 -H, OH are nootropic substances potent enhancers of learning processes and memory.

Orally or parenterally administrable pharmaceutical compositions in unit dosage form comprise between about 100 and about 500 mg of a compound of formula (1).

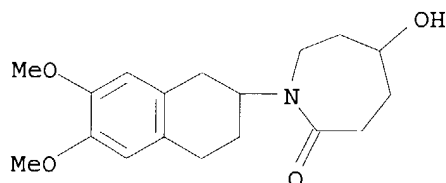
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT **143254-67-5P 143254-69-7P**

(preparation of)

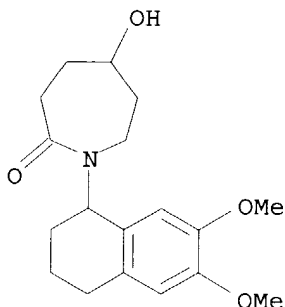
RN 143254-67-5 USPATFULL

CN 2H-Azepin-2-one, hexahydro-5-hydroxy-1-(1,2,3,4-tetrahydro-6,7-dimethoxy-2-naphthalenyl)- (9CI) (CA INDEX NAME)



RN 143254-69-7 USPATFULL

CN 2H-Azepin-2-one, hexahydro-5-hydroxy-1-(1,2,3,4-tetrahydro-6,7-dimethoxy-1-naphthalenyl)- (9CI) (CA INDEX NAME)



L95 ANSWER 25 OF 30 USPATFULL on STN

ACCESSION NUMBER: 87:50585 USPATFULL

TITLE: Substituted caprolactam derivatives as antihypertensives

INVENTOR(S): Harris, Elbert E., Westfield, NJ, United States
Patchett, Arthur A., Westfield, NJ, United States
Thorsett, Eugene D., Fanwood, NJ, United States

PATENT ASSIGNEE(S): Merck & Co., Inc., Rahway, NJ, United States (U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 4680392		19870714
APPLICATION INFO.:	US 1986-864234		19860519 (6)
RELATED APPLN. INFO.:	Continuation-in-part of Ser. No. US 1982-394749, filed on 2 Jul 1982, now patented, Pat. No. US 4629787 which is a continuation-in-part of Ser. No. US 1981-282580, filed on 13 Jul 1981, now abandoned which is a continuation-in-part of Ser. No. US 1980-179305, filed		

on 18 Aug 1980, now abandoned
DOCUMENT TYPE: Utility
FILE SEGMENT: Granted
PRIMARY EXAMINER: Bond, Robert T.
LEGAL REPRESENTATIVE: Mitri, Salvatore C., Sudol, Michael C., Monaco, Mario A.
NUMBER OF CLAIMS: 28
EXEMPLARY CLAIM: 1
LINE COUNT: 1662
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB The invention in its broad aspects relates to caprolactam derivatives which are useful as angiotensin converting enzyme inhibitors and as antihypertensives.

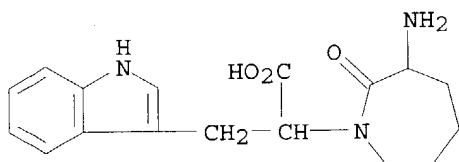
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 81867-57-4P

(preparation and alkylation of)

RN 81867-57-4 USPATFULL

CN 1H-Indole-3-propanoic acid, α -(3-aminohexahydro-2-oxo-1H-azepin-1-yl)- (9CI) (CA INDEX NAME)

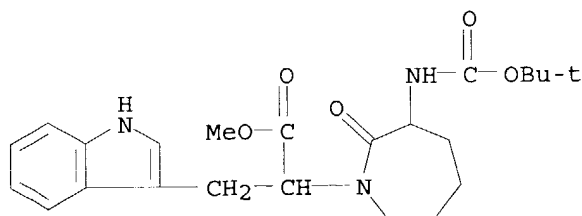


IT 81867-56-3P

(preparation and saponification of)

RN 81867-56-3 USPATFULL

CN 1H-Indole-3-propanoic acid, α -[3-[[[(1,1-dimethylethoxy)carbonyl]amino]hexahydro-2-oxo-1H-azepin-1-yl]-, methyl ester (9CI) (CA INDEX NAME)

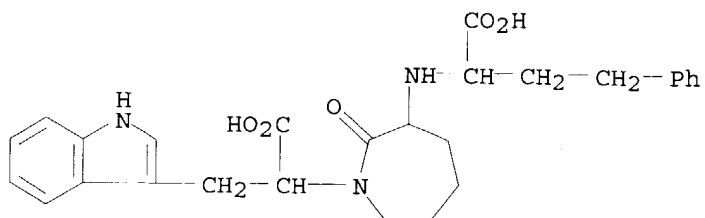


IT 81867-58-5P

(preparation of)

RN 81867-58-5 USPATFULL

CN 1H-Indole-3-propanoic acid, α -[3-[(1-carboxy-3-phenylpropyl)amino]hexahydro-2-oxo-1H-azepin-1-yl]- (9CI) (CA INDEX NAME)



L95 ANSWER 26 OF 30 USPATFULL on STN
 ACCESSION NUMBER: 86:71620 USPATFULL
 TITLE: Substituted caprolactam derivatives as antihypertensives
 INVENTOR(S): Harris, Elbert E., Westfield, NJ, United States
 Patchett, Arthur A., Westfield, NJ, United States
 Thorsett, Eugene D., Fanwood, NJ, United States
 PATENT ASSIGNEE(S): Merck & Co., Inc., Rahway, NJ, United States (U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 4629787		19861216
APPLICATION INFO.:	US 1982-394749		19820702 (6)
RELATED APPLN. INFO.:	Continuation-in-part of Ser. No. US 1981-282580, filed on 13 Jul 1981, now abandoned which is a continuation-in-part of Ser. No. US 1980-179305, filed on 18 Aug 1980, now abandoned		
DOCUMENT TYPE:	Utility		
FILE SEGMENT:	Granted		
PRIMARY EXAMINER:	Bond, Robert T.		
LEGAL REPRESENTATIVE:	Mitri, Salvatore C., Sudol, Michael C.		
NUMBER OF CLAIMS:	3		
EXEMPLARY CLAIM:	1		
LINE COUNT:	1484		

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
 AB The invention in its broad aspects relates to caprolactam derivatives which are useful as angiotensin converting enzyme inhibitors and as antihypertensives.

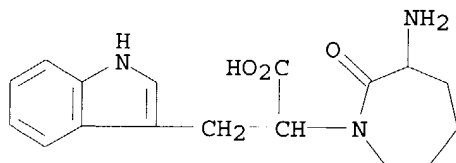
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT **81867-57-4P**

(preparation and alkylation of)

RN 81867-57-4 USPATFULL

CN 1H-Indole-3-propanoic acid, α -(3-aminoheptahydro-2-oxo-1H-azepin-1-yl)- (9CI) (CA INDEX NAME)

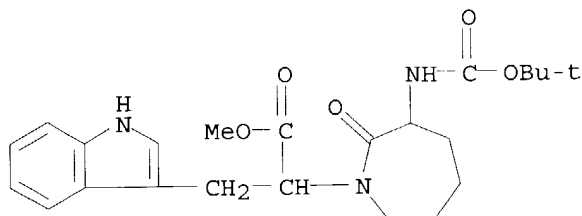


IT **81867-56-3P**

(preparation and saponification of)

RN 81867-56-3 USPATFULL

CN 1H-Indole-3-propanoic acid, α -[3-[[[(1,1-dimethylethoxy)carbonyl]amino]hexahydro-2-oxo-1H-azepin-1-yl]-, methyl ester (9CI) (CA INDEX NAME)

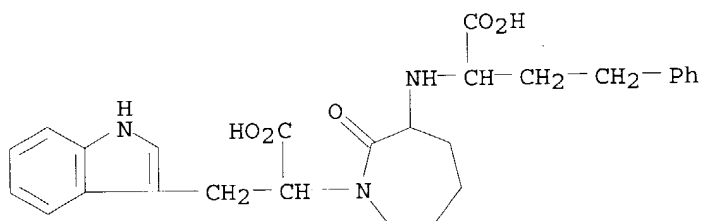


IT 81867-58-5P

(preparation of)

RN 81867-58-5 USPATFULL

CN 1H-Indole-3-propanoic acid, α -[3-[(1-carboxy-3-phenylpropyl)amino]hexahydro-2-oxo-1H-azepin-1-yl]- (9CI) (CA INDEX NAME)



L95 ANSWER 27 OF 30 TOXCENTER COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1978:91887 TOXCENTER

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DOCUMENT NUMBER: CA08905043156K

TITLE: Nitrosoarea derivatives

AUTHOR(S): Matsumoto, Jun; Murakami, Masuo; Sato, Noriaki; Hashimoto, Shinichi; Kawamura, Tsutomu; Ichikawa, Kaichiro

CORPORATE SOURCE: ASSIGNEE: Yamanouchi Pharmaceutical Co., Ltd.

PATENT INFORMATION: JP 7834790 31 Mar 1978

SOURCE: (1978) Jpn. Kokai Tokkyo Koho, 6 pp.

CODEN: JKXXAF.

COUNTRY: JAPAN

DOCUMENT TYPE: Patent

FILE SEGMENT: CAPLUS

OTHER SOURCE: CAPLUS 1978:443156

LANGUAGE: Japanese

ENTRY DATE: Entered STN: 20011116

Last Updated on STN: 20021210

AB Nitrosoarea derivs. I [R = 2-phenyl-2H-1,2,3-triazol-4-yl (II), 1-phenylpyrazol-5-yl, 4-methylphthalazan-3-yl, 1-adamantyl, 4-chloro-2-phenylpyrimidin-5-yl, Pr2NCO, 2,6-dioxopiperidin-4-ylmethyl, MeO2C] were prepared by silylation of III followed by reaction of RCOX (X = halo). I had antileukemic and anticarcinogenic activities (no data). Thus, 1.68 mL Et3N in dioxane was added to a mixture of 2.62 g III and 1.29 g Me3SiCl in dioxane, the whole stirred 20 h at room temperature, filtered, and

the filtrate concentrated to give 10 mL solution;
2-phenyl-1,2,3-triazol-4-carbonyl
chloride (1.5 g) in CH₂Cl₂ was added to 6 mL of the solution and the mixture
stirred 3 days at room temperature to give 165 mg II.

L95 ANSWER 28 OF 30 TOXCENTER COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1978:65668 TOXCENTER
COPYRIGHT: Copyright 2004 ACS
DOCUMENT NUMBER: CA08801006756Q
TITLE: Nitroso urea derivatives
AUTHOR(S): Murakami, Masuo; Ichikawa, Kaichiro; Matsumoto, Atsushi;
Sato, Norio; Hashimoto, Shinichi; Kawamura, Tsutomu
CORPORATE SOURCE: ASSIGNEE: Yamanouchi Pharmaceutical Co., Ltd.
PATENT INFORMATION: JP 7783747 12 Jul 1977
SOURCE: (1977) Jpn. Kokai Tokkyo Koho, 14 pp.
CODEN: JKXXAF.
COUNTRY: JAPAN
DOCUMENT TYPE: Patent
FILE SEGMENT: CAPLUS
OTHER SOURCE: CAPLUS 1978:6756
LANGUAGE: Japanese
ENTRY DATE: Entered STN: 20011116
Last Updated on STN: 20021210

AB Twenty-eight title derivs. I [R = halo, substituted alkyl,
(un)substituted alkenyl, (un)substituted aryl, (un)substituted
heterocyclics; n = 2-10] were prepared by reaction of II with RCOX (X =
halo). I had antitumor activity (some data given in mice). Thus, 174 mg
4-ClC₆H₄COCl in CHCl₃ was added to 440 mg 1-(β-chloroethyl)-3-(2-oxo-
3-hexahydroazepinyl)-1-nitroso-urea mercuric salt in CHCl₃ at room temperature
and the mixture stirred 3 h to give 204 mg 1-(β-chloroethyl)-3-(N-p-
chlorobenzoyl-2-oxo-3-hexahydroazepinyl)-1-nitroso-urea.

L95 ANSWER 29 OF 30 TOXCENTER COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1977:100440 TOXCENTER
COPYRIGHT: Copyright 2004 ACS
DOCUMENT NUMBER: CA08717135119N
TITLE: 1-(β-Chloroethyl)-3-substituted 1-nitroso-ureas
AUTHOR(S): Murakami, Masuo; Ichikawa, Kaichiro; Matsumoto, Jun; Sato,
Norio; Hashimoto, Shinichi; Kawamura, Tsutomu
CORPORATE SOURCE: ASSIGNEE: Yamanouchi Pharmaceutical Co., Ltd.
PATENT INFORMATION: JP 7751363 25 Apr 1977
SOURCE: (1977) Jpn. Kokai Tokkyo Koho, 10 pp.
CODEN: JKXXAF.
COUNTRY: JAPAN
DOCUMENT TYPE: Patent
FILE SEGMENT: CAPLUS
OTHER SOURCE: CAPLUS 1977:535119
LANGUAGE: Japanese
ENTRY DATE: Entered STN: 20011116
Last Updated on STN: 20021210

AB Thirteen title compds. (I, R = acyl) remedies for tumors, were prepared by
treating non-substituted I with a silylating agent followed by acylation.
Thus, 2.62 g 1-(β-chloroethyl)-3-(2-oxo-3-hexahydroazepinyl)-1-
nitroso-urea and Me₃SiCl in dioxane were treated with NEt₃ and treated with
352 mg p-[bis(β-chloroethyl)amino]benzoyl chloride in dichloromethane
to give 403 mg I [R = p-[bis(β-chloroethyl)amino]benzoyl]. Among 12
I similarly prepared were (R given): 4-oxo-4H-thiopyran-3-carbonyl,
p-O₂NC₆H₄CO, p-(dimethylamino)benzoyl, 3-methyl-2-oxo-2,3-
dihydrobenzothiazole-6-carbonyl.

L95 ANSWER 30 OF 30 TOXCENTER COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1977:96931 TOXCENTER
COPYRIGHT: Copyright 2004 ACS
DOCUMENT NUMBER: CA08713102197H
TITLE: Nitrosourea derivatives
AUTHOR(S): Murakami, Masuo; Ichikawa, Kaichiro; Matsumoto, Jun; Sato,
Norio; Hashimoto, Shinichi; Kawamura, Tsutomu
CORPORATE SOURCE: ASSIGNEE: Yamanouchi Pharmaceutical Co., Ltd.
PATENT INFORMATION: JP 7746072 12 Apr 1977
SOURCE: (1977) Jpn. Kokai Tokkyo Koho, 8 pp.
CODEN: JKXXAF.
COUNTRY: JAPAN
DOCUMENT TYPE: Patent
FILE SEGMENT: CAPLUS
OTHER SOURCE: CAPLUS 1977:502197
LANGUAGE: Japanese
ENTRY DATE: Entered STN: 20011116
Last Updated on STN: 20021210
AB Fifteen nitrosourea derivs. I [R1 = (un)substituted Ph, furyl, pyrazinyl,
H2C:CH, PhCH2, ClCH2, etc.] were prepared by reaction of II with R1COX (X =
halo). I had anticancer activity (some data given in mice). Thus, 124 mg
4-ClC6H4COCl in CHCl3 was added to 440 mg II HgCl2 salt in CHCl3 and the
mixture stirred 3 h at room temperature to give 204 mg I (R1 = 4-ClC6H4).

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FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Nov 26, 2004 (20041126/UP).

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